The quasicrystal model of cluster systems in condensed matter

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Abstract. The paper proposes a quasicrystal model of the structure of clusters. The model is based on the similarity of the structure of clusters and macroscopic structure of quasicrystals. It offers a formula to calculate the radii of successive coordination spheres in quasicrystalline films. The formula is based on the properties of Fibonacci sequence and characteristics of the power potential of interaction between particles.

1. Introduction

The structures of cluster systems and nanoscale objects are usually modeled by means of face-centered cubic (fcc), body-centered cubic (bcc) or hexagonal close packings of particles, with atoms in the cluster configuration corresponding to the volume of the sample structure. Even in an ideal crystal lattice of the cubic structure the model of close packing of hard spheres cannot describe the sequential arrangement of the coordination spheres in real crystals. The replacement of solid balls by soft spheres in the model has no notable effect on calculation results. Currently there are attempts to develop alternative models of cluster system structures.

Quasicrystal models of cluster structure are based on structural properties of quasicrystals. Quasicrystals are a large class of ordered materials occupying an intermediate position between classical crystals and amorphous substances. The first quasicrystal was discovered by Shechtman and colleagues in 1984 in the situation with the rapid cooling of the melt $\text{Al}_{86}\text{Mn}_{14}$ [1]. To date we know more than one hundred systems based on aluminum, gallium, copper, cadmium, nickel, titanium, tantalum, and other elements in which quasicrystals can form [2, 3].

Mathematical model of an ideal quasicrystal had been independently developed in two theories, that subsequently turned out to be equivalent. Levin and Steynardt [4] built a model of a quasicrystal based on two unit cells with an irrational ratio of their quantities. Certain construction rules, that are based Fibonacci series, lead to a structure without any periodicity in the arrangement of atoms, but with some properties that are typical of the crystal.

A common model of the structure of quasicrystalline objects is a two fragment model based on quasi-periodic covering of line, plane or space with two basic structural units. For one-dimensional quasicrystal this model leads to a Fibonacci series of short S and long L segments with $S = 1$ and $L = \Phi = 1.6180339 \ldots$. In the two-dimensional case the two fragment model is a Penrose tiling [5] composed of two types of rhombus with acute angles at the vertices $\pi/5$ and $2\pi/5$, in three-dimensional case it is the generalization of the Penrose tiling formed by rhombohedrons of two types and is called Amman-McKay network [2-5].
The model made by Kalugin, Kitaev and Levitova [6] is based on the "cubic" crystal in 6-dimensional space, which results in icosahedral quasicrystal. This crystal is used to cut out so-called "pipe", i.e. a layer of atoms that has the size of interatomic order and is concluded between three-dimensional hyperplanes. Then this pipe is projected onto physical space. Thanks to such arrangement it is possible to get continuum theory of the quasicrystal, to describe dislocations and clarify the nature of low-frequency collective modes.

Most of the existing theories of quasicrystal structuring are based on the idea of cluster approach to constructing aperiodic partitions. Within the framework of the cluster approach [7, 8] it is proved that quasicrystals are units of clusters. Their structure cannot be represented as a package of identical elementary cells. They present a unique packaging way of overlapping clusters, which allows us to realize the most stable and energetically favored local atomic configurations. Long-range order and extraordinary properties are caused by essentially localized fluctuations called phasons [7-9].

In the Penrose partition it is possible to distinguish two types of clusters made from three rhombs shaped that are shaped like a cube projection. These are either clusters made from two wide and one narrow rhombs, or an elongated clusters made of one wide and two narrow rhombs. Each rhomb is always a part of either one or two mutually overlapping clusters of these types [9]. Locally equivalent units of the same type are grouped together along the respective circumferences, the diameters of which differ by \( \Phi^\circ \) times. This feature allows us to draw an analogy with the circular property of linear fractional transformations (Möbius transformations) in the theory of functions of complex variables. Linear fractional transformation maps an arbitrary circle, that lies in the complex plane, into an equivalent circle, with direct lines regarded as circles of infinite radius. [9].

Dimensional model of the quasicrystal and Fibonacci series associated with the golden section are used to build a new type of optical elements: aperiodic gratings and multilayer structures [10-13]. Because of their unique physical properties the peculiarities of light diffraction on one-dimensional quasi-periodic structures (quasicrystals) have become the subject of various investigations in physics [10-13].

2. Quasicrystal model of cluster systems

In this paper we have adopted two fragment model based on the quasi-periodic covering of the space by two elementary structural units to be the basic model of the structure of cluster systems. In Penrose tiling model such elements are thin and thick rhombs with equal sides \( a \) with atoms of matter in their vertices. Thin rhomb has acute angle \( \frac{\pi}{5} = 36^\circ \), thick rhomb has acute angle \( \frac{2\pi}{5} = 72^\circ \). Atoms in the vertices of the thin rhomb form two dimers (see. Figure 1), similarly the atoms in the vertices of the thick rhomb form two other dimers

The first dimer is formed by the atoms of the thin rhomb with the centers of the masses of the atoms located at a distance equal to the rhomb small diagonal:

\[
R_{\text{dim}}^1 = 2a\sin \frac{\pi}{10} = a(\Phi - 1) = \frac{a}{\Phi} = 0.618...a
\]

the second dimer is formed by atoms lying at a distance of the long diagonal of the thin rhomb:

\[
R_{\text{dim}}^{\|} = 2a\cos \frac{\pi}{10} = a\sqrt{\Phi + 2} = 1.902...a
\]

and also

\[
R_{\text{dim}}^{\|} = R_{\text{dim}}^1 \cot \frac{\pi}{10} = R_{\text{dim}}^1 \Phi \sqrt{\Phi + 2} = 3.078...R_{\text{dim}}^1
\]

where \( \Phi = 1.6180339 \) - golden section constant.
The atoms in the vertices of the thick rhomb, like in the thin rhomb, form two more dimers with distances between the atoms $R_{\text{dim}}^{III}$ and $R_{\text{dim}}^{IV}$ respectively

$$R_{\text{dim}}^{III} = 2a \sin \frac{\pi}{5} = a \sqrt{3 - \Phi} = 1.175...a$$  \hspace{0.5cm} (4)

$$R_{\text{dim}}^{IV} = 2a \cos \frac{\pi}{5} = a \Phi = 1.618...a$$  \hspace{0.5cm} (5)

$$R_{\text{dim}}^{IV} = R_{\text{dim}}^{III} \cot \frac{\pi}{5} = R_{\text{dim}}^{III} \frac{\Phi}{\sqrt{3 - \Phi}} = 1.377...R_{\text{dim}}^{III}$$  \hspace{0.5cm} (6)

Figure 1. Golden rhombs pattern of the formation of atoms dimers in the structure of the cluster.

Each of four dimers makes the core of a forming cluster, so four types of clusters should be distinguished in this model and in X-ray electron diffraction analysis each of them demonstrates a diffraction pattern. General X-ray pattern is the result of superpositioning the four types of reflections that represent specific features of four types of clusters in the structure of the quasicrystalline system.

In the series of papers [14-17] the author et.al. have proposed a model of cluster formation in a disordered condensed media. According to this model the core of the cluster is a dimer around which a system of successive coordination spheres builds up. The result is the "shell structure" of a cluster. The appearance of defects in the shell structure of the cluster leads to unification and redistribution of the mutual arrangement of coordination spheres compared with the crystalline material phase and determines the temperature dependence of the coordination numbers in the cluster structure.

For a system of successive coordination spheres of spherical particles the radii of such spheres are represented by [16, 17]

$$R_n = R_{\text{dim}} \sqrt{p F_n}$$  \hspace{0.5cm} (7)

where $R_{\text{dim}}$ - the distance between the particles in each of the four dimers (1), (2), (4) and (5), $F_n$ - Fibonacci numbers, $p = 1, 2, 3, ...$ - natural numbers.

The rhomb side $a$ can be found by the formula (1), which $R_{\text{dim}}^{III}$ should be understood as the radius of the first coordination sphere. It is determined by the diameter of the matter particle and characteristics of the interaction potential [18].
\[ R_i = R_{\text{dam}} = \left( \frac{n}{m} \right)^{1-\sigma_0} \]  

(8)

where \( R_i \) - the radius of the first coordination sphere, \( \sigma_0 \) - the diameter of the sphere which simulates the atom, \( n > m \) - integers for Mie potential.

**Table 1.** The radii of successive coordination spheres in the structure of a quasicrystalline system measured in the units of \( a \).

| Fibonacci Numbers | 1  | 2  | 3  | 5  | 8  | 13 | 21 |
|-------------------|----|----|----|----|----|----|----|
| 0.618             | 0.874 | 1.070 | 1.382 | 1.748 | 2.228 | 2.832 |
| 1.175             | 1.662 | 2.035 | 2.627 | 3.323 | 4.236 | 5.385 |
| 1.618             | 2.288 | 2.802 | 3.618 | 4.576 | 5.834 | 7.415 |
| 1.902             | 2.690 | 3.294 | 4.253 | 5.380 | 6.858 | 8.716 |

**Table 2.** The radii of successive coordination spheres measured for the diamond film and macroscopic diamond.

| Number KS | \( R_n/a \) | \( R_n, \text{A} \) | \( R_n, \text{A} \) [19], Diamond film | \( R_n, \text{A} \) [20], Bulk diamond |
|-----------|-------------|-----------------|--------------------------------------|--------------------------------------|
| 1         | 0.618       | 1.73            | 1.44                                 | 1.544 (111)                          |
| 2         | 0.874       | 2.45            | 2.48                                 | 2.522 (220)                          |
| 3         | 1.070       | 3.00            | 2.96                                 | 2.957 (311)                          |
| 4         | 1.175       | 3.29            | 3.30                                 | 3.566 (400)                          |
| 5         | 1.382       | 3.88            | 3.70                                 | 3.886 (331)                          |
| 6         | 1.618       | 4.54            | –                                    | 4.368 (422)                          |
| 7         | 1.748       | 4.90            | 5.11                                 | 4.633 (333)                          |
| 8         | 1.902       | 5.33            | –                                    | 5.044 (440)                          |
| 9         | 2.035       | 5.71            | 5.96                                 | 5.847 (533)                          |
| 10        | 2.228       | 6.25            | –                                    | 6.367 (551)                          |
| 11 KS     |             |                 |                                       | 13 KS                                |
| 12 KS     |             |                 |                                       | 13 KS                                |
| 13 KS     |             |                 |                                       | 13 KS                                |
| 14 KS     |             |                 |                                       | 13 KS                                |
| 15        | 2.815       | 7.89            | 7.80                                 | 7.975 (840)                          |
| 16        | 3.315       | 9.30            | 8.80                                 | 9.223 (773)                          |
| 17        | 3.615       | 10.14           | 10.2                                 | 10.205 (955)                         |
| 18        |             |                 |                                       | 33 KS                                |
Taking into account the said assumptions, the rhomb side will be determined by the formula

\[ a = \Phi \left( \frac{n}{m} \right)^{\frac{1}{m-n}} \sigma_0 \]  

(9)

Now let’s calculate the radii of coordination spheres for carbon films. The diameter of carbon atoms is \( \sigma_0 = 1.544 \text{Å} \), so for the Lennard-Jones potential \((m = 6, n = 12)\) the rhomb side will be \( a = 2^6 \Phi \sigma_0 = 2.804 \text{Å} \). Considering Table 1 and placing the radii of coordination spheres in monotonic increase order we’ll obtain absolute values of the radii of coordination spheres with the rhomb side size \( a = 2.804 \text{Å} \).

Table 2 calculation data on the radii of successive coordination spheres for the diamond film consisting of two-dimensional Fibonacci clusters. These results, obtained by the proposed calculation method, are compared with X-ray diffraction data for diamond films [19] and the results of theoretical calculations for bulk diamonds [20].

As the proposed cluster model resulted in obtaining the values of the radii of the first six coordination spheres that are in good agreement with the results of X-ray diffraction patterns in amorphous carbon films [19] and have just a small offset from the radii of coordination spheres in the crystal macroscopic diamond [20], the short-range ordering (within five coordination spheres) in tightly packed carbon systems can be simulated by means of quasicrystal models.

3. Conclusion

Quasicrystal models of the structure of cluster systems in the structure of carbon films can be used to predict the position of coordination spheres consistently with the results of X-ray diffraction measurements. Successive arrangement of coordination is explained by peculiarities of Fibonacci series and the golden section. Carbon films form up from quasicrystalline clusters according to the principle of the close packing of golden rhombs, which is mathematically expressed by the following rule: the radius of the n-th coordination sphere is proportional to the square root of the corresponding Fibonacci number.

The determining parameter of the model is the side of golden rhombs; it depends on the diameter of the matter particles and the nature of the interaction between particles. In case of Mie power potential it depends on the exponent in the repulsive and attractive parts of the potential.

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