Quantum dots in the structure of quasicrystalline systems

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Abstract. The article shows that in the structure of quasicrystalline systems it is possible the formation of quantum dots, which are potential wells of various forms with quantized motion of an electron or proton, which allowed us to put forward the hypothesis of the existence of a constant component in the infrared radiation of the moon surface.

1. Introduction
Quasicrystals are a large class of ordered substances that occupy intermediate position between classical crystals and amorphous substances. The first quasicrystal obtained by rapid cooling of Al₀.₈₆Mn₀.₁₄ alloy was discovered by D. Shechtman et al in 1984 [1]. For the discovery of a new class of solids Schechtman in 2011 was awarded the Nobel Prize in Chemistry.

To date, more than a hundred systems based on aluminum, gallium, copper, cadmium, nickel, titanium, tantalum and other elements in which quasicrystals are formed [1–3]. There are several principles for constructing quasicrystalline systems, one of which, for quasicrystalline films, is based on the principles of the "golden section". Can suggest the appearance of quasicrystalline films under certain conditions and on surfaces of some multiferroics and ferromagnets [20].

2. The formation of quasicrystalline films on the principles of the "golden section"
The basis of the model of the structure of cluster film systems, adopted by the authors [4–7, 20] is two-fragment model based on quasiperiodic coverage of space by two elementary structural units. As part of the Penrose parquet model, such the elements are thin and thick rhombuses with equal sides $a$, at the vertices of which are atoms of matter. Thin rhombus has an acute angle $\frac{\pi}{5} = 36^\circ$, a thick rhombus with acute angle $2\pi/5 = 72^\circ$. Atoms located at the vertices of a thin rhombus form two dimers, similarly the atoms at the vertices of a thick rhombus form two more dimers (figure 1).

The defining parameter of the model is the side of the “golden” rhombuses, depending on particle diameter of the substance and the nature of the interaction between the particles. In the case of a power law Mi potential [8–11]:

$$U(r) = \frac{\epsilon_0}{n-m} \left[ m \left( \frac{\sigma_0}{r} \right)^n - R \left( \frac{\sigma_0}{r} \right)^m \right],$$

where $m, n$ — are dimensionless interaction parameters, $\epsilon_0$ — is the binding energy, $\sigma_0$ — is the length bonds — effective particle diameter, $r$ — equilibrium distance between two atoms, the side of the rhombuses depends on the degree indicators in the attracting and repelling parts interaction potential (1).
We will consider the radii of atoms as half the radii of the first coordination spheres radial distribution function for a pure substance. For atomic radii according to Figure 1 for two types of atoms, we write [8–11]:

\[
\begin{align*}
    r_1 &= \frac{R_1}{2} = \frac{1}{2} \left( \frac{n_1}{6} \right)^{1/6} \sigma_{01}, \\
    r_2 &= \frac{R_2}{2} = \frac{1}{2} \left( \frac{n_2}{6} \right)^{1/6} \sigma_{02},
\end{align*}
\]

where it is assumed that ratio (2) corresponds to the dispersion forces of attraction.

Condition \( r_1 > r_2 \), taking into account the properties of the “golden” rhombus, we find the condition most dense packaging for particles of two varieties, the radii of which are connected according to Figure 1 trigonometric functions of the "golden" angles (table 1).

**Table 1.** Trigonometric functions of the "golden" angles.

| Function | \( \pi/10 = 18^\circ \) | \( \pi/5 = 36^\circ \) | \( 3\pi/10 = 54^\circ \) | \( 2\pi/5 = 72^\circ \) | \( 3\pi/5 = 108^\circ \) |
|----------|-----------------|-----------------|-----------------|-----------------|-----------------|
| \( 2\sin \alpha \) | \( \Phi - 1 \) | \( \sqrt{3} - \Phi \) | \( \Phi \) | \( \sqrt{\Phi + 2} \) | \( \sqrt{3} + \Phi \) |
| \( 2\cos \alpha \) | \( \sqrt{\Phi + 2} \) | \( \Phi \) | \( \sqrt{3} - \Phi \) | \( \Phi - 1 \) | \( 1 - \Phi \) |
| \( r_2/r_1 \) | 2.236 | 0.7013 | 0.2361 | 0.05146 | 0.05146 |

Where \( \Phi = 1.618 \ldots \) — is the golden ratio.

The most dense packing condition for particles of two varieties whose radii are connected trigonometric functions of the “golden” angles (table 1), is written in the form [8–11]:

\[
r_2 = r_1 \left( \frac{2}{2\sin \alpha} - 1 \right).
\] (3)

We give an example. The radius of the fluorine atom is \( r_1(F) = 0.7013 \) Å, consequently, according to table 1 and figure 1 most preferred for the formation of dense packings of atoms in a thin film will be atoms of a different kind with radii: \( r_2 = 1.63 \) Å; \( 0.51 \) Å; \( 0.172 \) Å.

The radius of the magnesium atom \( r_2(Mg) = 1.60 \) Å in combination with a fluorine atom can form a "golden" rhombus with a corner \( \pi/5 = 36^\circ \). Such a compound exists — it is magnesium fluoride (MgF\(_2\)), which is, under normal conditions, colorless diamagnetic tetrahedral crystals with space group \( P4/mnm(a = 4.625 \) Å, \( c = 3.052 \) Å, \( Z = 2) \).

Second value \( r_2 = 0.51 \) Å close to the radius of the hydrogen atom to form a compound hydrogen fluoride (HF) — a colorless gas (under standard conditions) with a pungent odor, when room temperature exists mainly in the form of a dimer \( H_2F_2 \), below 19.9 °C — colorless mobile fluid.
Miscible with water in any respect to form hydrofluoric (hydrofluoric) acid. Hydrogen fluoride in liquid and gaseous states has a high propensity for association due to the formation of strong hydrogen bonds. The energy of hydrogen bonds $\text{FH} \cdots \text{HF}$ is approximately $42 \text{kJ/mol}$. Even in the gaseous state of hydrogen fluoride consists of a mixture of $\text{H}_2\text{F}_2$, $\text{H}_3\text{F}_3$, $\text{H}_4\text{F}_4$, $\text{H}_5\text{F}_5$, $\text{H}_6\text{F}_6$. Simple HF molecules exist only at temperatures above 90 $^\circ\text{C}$. Due to its high strength the thermal decomposition of hydrogen fluoride becomes noticeable only above 3500 $^\circ\text{C}$ (which is higher the melting point of tungsten — the most refractory of metals).

In the crystalline state HF forms orthorhombic crystals consisting of chain-like structures: angle $\angle\text{HFH} = 116^\circ$, bond length $l_{(\text{F-H})} = 0.95$ Å, $l_{(\text{F-H})} = 1.55$ Å. Similar zigzag chains with an angle $\angle\text{HFH} = 140^\circ$ have polymers HF, existing in the gas phase (figure 2).

![Polymer chains in the structure of hydrogen fluoride](image)

**Figure 2.** Polymer chains in the structure of hydrogen fluoride

3. Quantum dots as two-dimensional potential wells

Eigenvalues of the energy of a particle located at the $n$ energy level in potential well are determined by the formula [13]:

$$E_n = \frac{\pi^2\hbar^2}{2ml^2}, \quad (n = 1, 2, 3, ...),$$

where $l$ — is the width of the potential well, $m$ — is the mass of the particle, $\hbar = 1.05 \cdot 10^{-34}$ J$\cdot$s — Planck’s constant.

$$\Delta E_{n+1,n} = \frac{\pi^2\hbar^2}{2ml^2} (2n + 1), \quad (n = 1, 2, 3, ...).$$

For small values of $n$ the discrete character of the energy spectrum appears, for large $n$ discrete character is smoothed out and the energy spectrum becomes continuous. For example, when $n = 3$ formula (5) gives a result of 0.78, for $n = 10$ we get 0.21, at $n \to \infty$, $E \to 0$. For small values of $n$ the equality $(2n + 1) = F_i$, $F_i$ — Fibonacci numbers, then based on formulas (4) and (5) we write:

$$\omega_n = \frac{\hbar}{h} \Delta E_{n+1,n} = \frac{\pi^2\hbar}{2ml^2} \cdot (\Phi - 1)F_i, \quad (l = 1, 2, 3, ...).$$

At $F_i = 1$ on the basis of formula (6) for the wave vector we get:

$$\left(\frac{\omega_n}{c}\right) = \frac{1}{\hbar - \omega_n} \Delta E_{n+1,n} = \frac{\pi^2\hbar}{2mc^2l^2} \cdot (\Phi - 1), \quad \text{cm}^{-1}.$$  

In formula (7), the mass of a particle is usually understood as the mass of an electron, then radiation from the quantum dot lies in the region of ultraviolet frequencies. For rectangular potential pit wide $l = 0.67$ Å by the formula (7) we get:

$$\left(\frac{\omega_n}{c}\right) = \frac{1}{\hbar - \omega_n} \Delta E_{n+1,n} = 3.6 \cdot 10^6 \text{ cm}^{-1}; \quad \lambda = 0.0174 \mu\text{m}.$$

If the proton is in the quantum dot, similarly to formula (8), we obtain:

$$\left(\frac{\omega_n}{c}\right) = \frac{1}{\hbar - \omega_n} \Delta E_{n+1,n} = \frac{\pi^2\hbar}{2m_pcl^2} \cdot (\Phi - 1) = 1750 \text{ cm}^{-1}.$$  

This frequency value corresponds to the wavelength $\lambda = 35.9$ $\mu$m, i.e. the radiation lies in infrared spectrum.
Potential wells, whose properties are determined by ratios (5)–(9), can treat as quantum dots emitting electromagnetic waves of a certain frequency. We note that protons in the structure of quantum dots can appear as a result of proton exchange processes, or as a result of proton-ion modification crystals and glasses used to obtain homogeneous surface layers with expressed internal interface with bulk material [15, 16].

In the framework of the proposed model, using ratios (2), (3) and (8), it is possible to describe basic laws of proton-ion implantation processes.

Proton implantation is usually carried out on a cyclotron (for example, on a U-120 cyclotron FTI Tomsk PU). The proton component in pulses of ~ 2 ns duration was more than 40 %. The current and beam energy were respectively 100 mA/cm² and 120 Kev. At exposure of LiNbO₃ X-crystals to a direct proton flux damage networks with a period of 10–30 µm, due to the emergence of planes on the surface cleavage. When the number of pulses is more than 8, the destruction of crystals with the formation of deep microcracks (~150–200 µm) [15, 16].

4. The radiation of the lunar surface in the infrared range

The proposed approach for the formation of quantum dots in quasicrystalline films allows you to put forward a hypothesis on the formation of infrared radiation on the surface of the moon.

Table 2. The formation of quasicrystalline systems of the lunar surface [15, 16, 18, 19].

| Lunar Element soil (Luna-20) | Quasicrystalline system, $r_1$ (Å) [12] |
|-----------------------------|---------------------------------------|
| Silicon (Si), 23 % $r_1$ = 1.32 Å | $r_1$ = 0.92 Å **Sulfur Silicon Sulphide** — Binary Inorganic a compound of silicon and sulfur with the formula SiS₂, white or gray crystals, easily hydrolyzed by water, reacts with atmospheric oxygen. |
| Iron (Fe), 13 % $r_1$ = 1.56 Å | $r_1$ = 1.09 Å **Phosphorus**. Iron-phosphorus alloys obtained and used to restore and increase the wear resistance of machine parts. The books [18, 19] describe classical methods for producing alloys iron with phosphorus (ferrophosphorus). |
| Calcium (Ca), 10 % $r_1$ = 1.94 Å | $r_1$ = 1.35 Å **Gallium**. The CaGa compound has an orthorhombic lattice with parameters $a = 0.4382$ nm, $b = 1.1935$ nm, $c = 0.4196$ nm. The low-temperature modification of CaGa₂ has a hexagonal grid with parameters $a = 0.4461$ nm, $c = 0.7359$ nm. Tetragonal a lattice is observed for compound CaGa₄ with parameters $a = 0.4365$ nm, $c = 1.065$ nm. Compound Ca₂₈Ga₁₁ has a complex structure consisting of the three types of polyhedra with Ca atoms around Ga atoms. |
| Aluminum (Al), 12.5 % $r_1$ = 1.18 Å | $r_1$ = 0.83 Å **Chlorine. Aluminum chloride** — colorless crystals, fuming due to hydrolysis in moist air. At normal pressure sublimes at 183 °C (melts under pressure at 192.6 °C). In water soluble (44.38 g in 100 g H₂O at 25 °C). From aqueous solutions crystalline hydrate AlCl₃·6H₂O precipitates - yellowish white fuzzy crystals. Soluble in many organic compounds (in ethanol — 100 g in 100 g of alcohol at 25 °C; in acetone, 1,2-dichloroethane, ethylene glycol, nitrobenzene, carbon tetrachloride, etc.); however, it is practically insoluble in benzene and toluene. And compound with strontium [14]. |
| Magnesium (Mg), 5.7 % $r_1$ = 1.45 Å | $r_1$ = 1.01 Å **Phosphorus. Magnesium Phosphide** — Binary Inorganic a compound of magnesium and phosphorus with the formula Mg₃P₂. Bright yellow cubic crystals. |
| Fluorine (F), 5.1 % $r_1$ = 0.42 Å | $r_1$ = 0.29 Å **Helium**. Researchers conducted a large-scale search possible stable helium compounds with various elements (H, O, F, Na, K, Mg, Li, Rb, Cs, etc.) using the USPEX code (Universal Structure Predictor: Evolutionary Xtallography), developed by Oganov and by his colleagues in 2004 [18, 19]. |
The lunar surface is constantly exposed to the solar wind, representing flows of ionized particles. The solar wind is quite variable. Thanks to processes occurring inside the star, it can have different intensities and speed. The solar wind can be calm and indignant. Calm flows the solar wind can be divided into two types: slow and fast. Slow possess speeds of about 300–500 km/s. They form in the calm parts of the corona of the Sun. Fast flows have a speed of 500 to 800 km/s. They are formed largely due to the existence of coronal holes in the Sun — areas in the solar corona, where the density and the temperature are noticeably lower than in other parts of the crown.

In total, calm flux accounts for 53% of the solar radiation time. Most a common cause of disturbed flows is the ejection of particles from the solar corona (so called coronal mass ejection). It is interesting in that the huge masses of plasma (protons, electrons, and some ions of heavy elements) are emitted from the corona with tremendous speed, since almost all the energy of the ejection is spent on the acceleration of these particles.

The energy spectrum of solar wind particles is quite wide, so there are always proton-ion flows corresponding to the implantation conditions of solar wind particles in the structure of the substances of the lunar surface and the formation of quantum dots emitting electromagnetic waves in the infrared range.

Moon radiation in the infrared is stable and constant in time and space. The basis of digital models of the radiation temperature of the moon are physical laws and statistical relationships between the intensity of thermal and reflected radiation, geometric parameters, the albedo value and the lunar microstructure surface. A computer image of the infrared moon is used to radiometric calibration of on-board artificial meteorological equipment satellites [17].

5. Findings
1. When irradiating a metal surface with proton-ion fluxes at a certain the ratio of the diameters of the atoms of the irradiated metal and the ions of the irradiating flow on a quasicrystalline film with densest packing forms on the surface of the metal atoms. In the structure of a quasicrystalline film, atom-free regions form about 1 Å in size, which are traps for protons from the irradiating stream, thus, a quantum dot appears.

The atomic packing of a quasicrystalline film is a packing of equilateral Penrose rhombuses at the peaks, which are atoms of two varieties.

2. Application of the laws of proton-ion implantation processes for interaction solar wind with the lunar surface hypothesized the existence of IR radiation of the moon due to quasicrystalline emission of quantum dots rock structures of the lunar surface.

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