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MODELING QUASI-LATTICE WITH OCTAGONAL SYMMETRY

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We prove the possibility to use the method of modeling of a quasi-lattice with octagonal symmetry similar to that proposed earlier for the decagonal quasicrystal. The method is based on the multiplication of the groups of basis sites according to specified rules. This model is shown to be equivalent to the method of the periodic lattice projection, but is simpler because it considers merely two-dimensional site groups. The application of the proposed modeling procedure to the reciprocal lattice of octagonal quasicrystals shows a fairly good matching with the electron diffraction pattern. Similarly to the decagonal quasicrystals, the possibility of three-index labeling of the diffraction reflections is exhibited in this case. Moreover, the ascertained ratio of indices provides information on the intensity of diffraction reflections.

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1. INTRODUCTION

The description of the quasicrystalline phase structure is a nontrivial problem of material science. This is a consequence of the impossibility to select a unit cell reflecting the overall structure of a lattice [1–5]. Different approaches and methods possessing both the virtues and shortcomings are commonly used for this. For example, we note the Ammann–Beenker tiling, which is an eight-fold sibling of the more famous, five-fold Penrose rhombus tiling [6, 7], and the Burkov method [1], which consists in structure constructing with overlapping clusters. Unfortunately, essential difficulties arise in indexing the diffraction patterns from such phases. In this case, it is necessary to use more than three basis vectors, and moreover, the number of vectors depends on a symmetry of the quasilattice. For example, in the case of icosahedral quasicrystals, six basis vectors could be used [8–10], whereas in the case of a decagonal quasilattice, the number of basis vectors is five or six [11]. Accordingly, more than three indices should be used for the diffraction reflection indexing. The feasible values of these indices are not quite obvious, because the limitations specified by the quasilattice symmetry should be held. In terms of the projection method, which is often used for the modeling of quasi-lattices [12, 13], this limitation is, evidently, equivalent to forbidding projection of the sites of a periodic hyper-lattice with the dimension higher than three, which are sufficiently far from the physical space. Thus, the complications related to both the identification and indexing of the reflection arise. It should be noted that the method of solving the above problem using only two indices (N, M) is now well developed [14]. The indexing procedure of the diffraction reflections for decagonal quasicrystals using three indices was proposed in Ref. [15]. A similar procedure of indexing for other types of quasicrystalline phases (octagonal and dodecagonal) has not yet been considered. Therefore, the aim of this work is the generalization and extension of the approach developed previously for icosahedral and decagonal quasilattices to other types of quasicrystals, in particular, those possessing octagonal symmetry.

2. MODELING THE QUASI-LATTICE WITH OCTAGONAL SYMMETRY

The method of modeling a quasicrystalline lattice with a tenfold axis of symmetry has been proposed and described in detail in Ref. [15]. This method consists in the multiplication of geometric groups (sites) according

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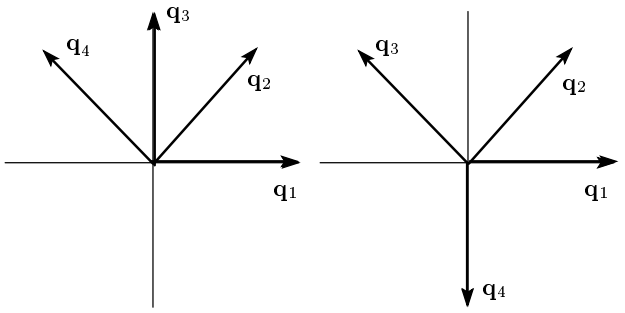

Fig. 1. The variants of choosing the basis vectors

to one of the three possible algorithms. These algorithms could be formally expressed as $D_n = D_{n-1} + \{\tau^{n-2}\mathbf{q}_i\}D_{n-2}$, $D_n = D_{n-2} + \{\tau^{n-2}\mathbf{q}_i\}D_{n-1}$, and $D_n = D_{n-1} + \{\tau^{n-2}\mathbf{q}_i\}D_{n-1}$. Here, D_n is a geometric group of sites of n; the order $\mathbf{q}_i$ is a set of ($\pm\mathbf{q}_1$, $\pm\mathbf{q}_2$, $\pm\mathbf{q}_3$, $\pm\mathbf{q}_4$, $\pm\mathbf{q}_5$) vectors, which are the vertices of a regular decagon; the expression $D_n = D_{n-1} + \{\tau^{n-2}\mathbf{q}_i\}D_{n-1}$ corresponds to adding the geometric groups shifted by the $\tau^{n-2}\mathbf{q}_i$ vectors to a preceding geometric group; and $\tau = 2\cos(\pi/5) = (1+\sqrt{5})/2$ is the irrational number expressing the so-called "golden ratio".

We show that this algorithm is applicable to quasicrystalline lattices of the octagonal symmetry. In this case, the system of basis vectors can be specified by two methods differing by the mutual orientation of four basis vectors (Fig. 1):

$$\begin{aligned} \mathbf{q}_1 &= (1\mathbf{i} + 0\mathbf{j}), \quad \mathbf{q}_2 = \left(\frac{\sqrt{2}}{2}\,\mathbf{i} + \frac{\sqrt{2}}{2}\,\mathbf{j}\right), \\ \mathbf{q}_3 &= (0\mathbf{i} + 1\mathbf{j}), \quad \mathbf{q}_4 = \left(-\frac{\sqrt{2}}{2}\,\mathbf{i} + \frac{\sqrt{2}}{2}\,\mathbf{j}\right) \end{aligned} \tag{1}$$

and

$$\begin{aligned} \mathbf{q}_1 &= (1\mathbf{i} + 0\mathbf{j}), \quad \mathbf{q}_2 = \left(\frac{\sqrt{2}}{2}\,\mathbf{i} + \frac{\sqrt{2}}{2}\,\mathbf{j}\right), \\ \mathbf{q}_3 &= \left(-\frac{\sqrt{2}}{2}\,\mathbf{i} + \frac{\sqrt{2}}{2}\,\mathbf{j}\right), \quad \mathbf{q}_4 = (0\mathbf{i} - 1\mathbf{j}). \end{aligned} \tag{2}$$

Hence, an ambiguity in the selection of a basis arises. Accordingly, if $\mathbf{q}_i$ are considered as the reciprocal lattice vectors, then indexing the diffraction reflections for an octagonal quasicrystal is also ambiguous. For definiteness, system (1) is adopted as a basis.

If the system of $\mathbf{q}_i$ vectors ($\pm\mathbf{q}_1$, $\pm\mathbf{q}_2$, $\pm\mathbf{q}_3$, $\pm\mathbf{q}_4$) is chosen as the initial geometric group O_1, it is possible to express the algorithm of lattice construction in the form

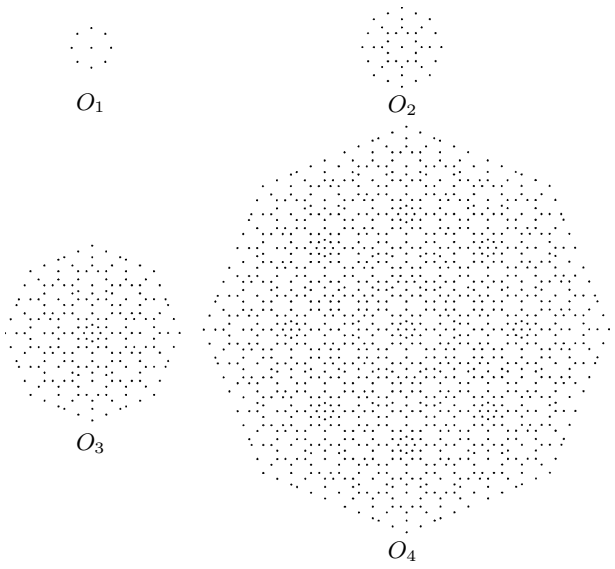

Fig. 2. Illustration of the geometry groups, construction in the case of an octagonal lattice

$$O_2 = O_1 + \{\mathbf{q}_i\}O_1, \quad O_n = O_{n-1} + \{\delta_s^{n-2}\mathbf{q}_i\}O_{n-1}. \tag{3}$$

Here, we use the irrational number $\delta_s = 1 + \sqrt{2}$, known as "silver ratio", as a counterpart for the "golden ratio" τ [16]. One of the features of the silver ratio is that it allows expressing the powers of δ_s in the form

$$\delta_s^n = K_n\delta_s + K_{n-1}, \tag{4}$$

where K_n are the Pell's numbers (0, 1; 2; 5; 12; 29; 70; 169; 408; ...) satisfying the condition $K_n = 2K_{n-1} + K_{n-2}$ [17].

We emphasize that the following relation between the basis vectors (1) exists:

$$\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3 = \delta_s\mathbf{q}_2. \tag{5}$$

With Eqs. (4) and (5), we can write

$$\begin{aligned} \delta_s^n\mathbf{q}_2 &= K_n(\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3) + K_{n-1}\mathbf{q}_2 = \\ &= \hat{E}_n(\mathbf{q}_1 + \mathbf{q}_3)(K_n + \hat{E}_{n-1})\mathbf{q}_2. \end{aligned} \tag{6}$$

Thus, any site of the $O_n = O_{n-1} + \{\delta_s^{n-2}\mathbf{q}_i\}O_{n-1}$ geometric group can, evidently, be expressed as a linear combination of the basis vectors in the form $\mathbf{Q} = n_1\mathbf{q}_1 + n_2\mathbf{q}_2 + n_3\mathbf{q}_3 + n_4\mathbf{q}_4$. The application of this algorithm to the O_4 geometric group is illustrated in Fig. 2.

We note that algorithm (3) of the construction of a quasi-periodic lattice with an eightfold symmetry axis can be modified by substituting one or several

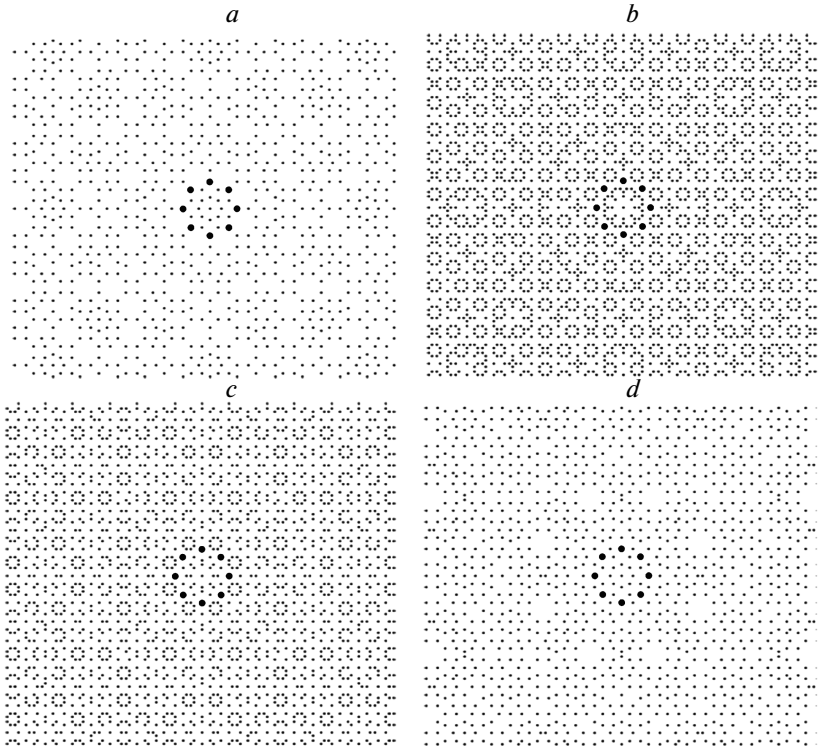

Fig. 3. Fragments of the octagonal lattices constructed according to different algorithms (the O_1 group is distinguished): *a*) $O_2 = O_1 + \{\mathbf{q}_i\}O_1$, $O_n = O_{n-1} + \{\delta_s^{n-2}\mathbf{q}_i\}O_{n-1}$; *b*) $O_2 = O_1 + \{\mathbf{q}_i\}O_1$, $O_3 = O_2 + \{\mathbf{2q}_i\}O_2$, $O_n = O_{n-1} + \{\delta_s^{n-3}\mathbf{q}_i\}O_{n-1}$; *c*) $O_2 = O_1 + \{\mathbf{q}_i\}O_1$, $O_3 = O_2 + \{\sqrt{\mathbf{2}}\mathbf{q}_i\}O_2$, $O_n = O_{n-1} + \{\delta_s^{n-3}\mathbf{q}_i\}O_{n-1}$; *d*) $O_2 = O_1 + \{\sqrt{\mathbf{2}}\mathbf{q}_i\}O_1$, $O_n = O_{n-1} + \{\delta_s^{n-2}\mathbf{q}_i\}O_{n-1}$

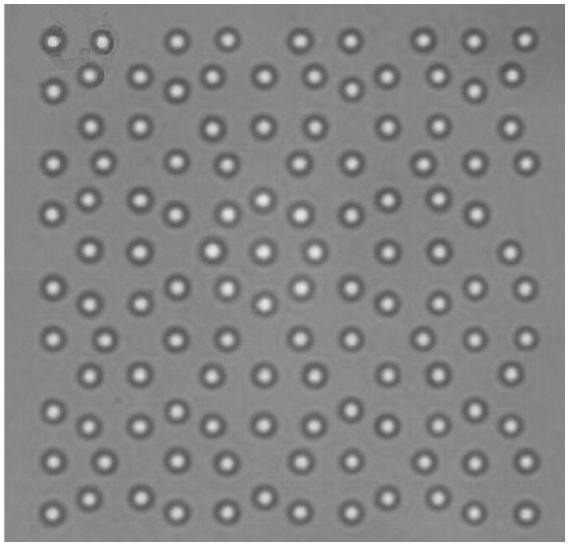

Fig. 4. Two-dimensional colloidal quasicrystals organized with holographic optical traps [18]

numerical coefficients (Fig. 3). It is important that this coefficient is expressed in terms of a relation between the basis vectors similar to Eq. (5). In contrast to the known methods of modeling [1, 5–7, 11, 13], this method for multiplying groups of nodes allows classifying the quasicrystalline structures. For example, a two-dimensional dielectric quasicrystalline heterostructure is shown in Fig. 4 [18]. It is evident that this structure corresponds to the model shown in Fig. 3*d*. This structure can be assigned to type $O(\delta_s - 1, \delta_s^{n-2})$, according to the numerical coefficients involved in the algorithm. The structures obtained for other algorithms (Fig. 3*a*,*b*,*c*) can be denoted as $O(1, \delta_s^{n-2})$, $O(1, 2, \delta_s^{n-3})$, and $O(1, \delta_s - 1, \delta_s^{n-3})$. It is easily seen that the algorithm changes; for example, the coefficients in $O_2 = O_1 + \{\delta_s\mathbf{q}_i\}O_1$, $O_3 = O_2 + \{\mathbf{q}_i\}O_2$, $O_4 = O_3 + \{\mathbf{2q}_i\}O_3$, and $O_n = O_{n-1} + \{\delta_s^{n-3}\mathbf{q}_i\}O_{n-1}$ can be reduced to the construction of structures such as $O_2 = O_1 + \{\mathbf{q}_i\}O_1$, $O_3 = O_2 + \{\mathbf{2q}_i\}O_2$, and $O_n = O_{n-1} + \{\delta_s^{n-3}\mathbf{q}_i\}O_{n-1}$. Hence, it is advisable to write the coefficients in the notation for the structural class in ascending order.

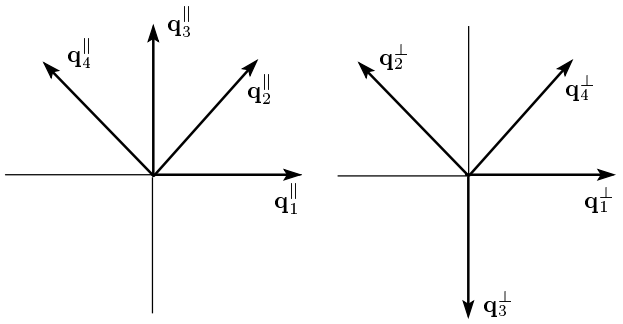

Fig. 5. Mutual orientation of the basis vector projections in the physical and perpendicular spaces

It is known [5, 19] that a quasicrystalline lattice can be represented in terms of the projection of a periodic lattice in a space of dimension R onto the space of a lower dimension d. In the case of an octagonal planar lattice, the projection of the four-dimensional cubic lattice onto the plane can be proposed. If the basis of the four-dimensional lattice is represented in a form of orthogonal vectors

$$\begin{aligned} &\mathbf{u}_1 = [1\,0\,1\,0], \quad \mathbf{u}_2 = \left[\frac{\sqrt{2}}{2}\,\frac{\sqrt{2}}{2}\,-\frac{\sqrt{2}}{2}\,\frac{\sqrt{2}}{2}\right], \\ &\mathbf{u}_3 = [0\,1\,0\,-1], \quad \mathbf{u}_4 = \left[-\frac{\sqrt{2}}{2}\,\frac{\sqrt{2}}{2}\,\frac{\sqrt{2}}{2}\,\frac{\sqrt{2}}{2}\right], \end{aligned} \tag{7}$$

then the first two coordinates of each vectors correspond to basis vectors (1). The other two coordinates correspond to the vectors

$$\begin{aligned} &\mathbf{q}_1^{\perp} = (1\mathbf{i} + 0\mathbf{j}), \quad \mathbf{q}_2^{\perp} = \left(-\frac{\sqrt{2}}{2}\,\mathbf{i} + \frac{\sqrt{2}}{2}\,\mathbf{j}\right), \\ &\mathbf{q}_3^{\perp} = (0\mathbf{i} - 1\mathbf{j}), \quad \mathbf{q}_4^{\perp} = \left(-\frac{\sqrt{2}}{2}\,\mathbf{i} + \frac{\sqrt{2}}{2}\,\mathbf{j}\right), \end{aligned} \tag{8}$$

which are the projections of system (7) onto a perpendicular space. Mutual orientation of the basis vectors in the perpendicular space for the selected basis (1) in the physical space is presented in Fig. 5. Evidently, the vector $\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3$ in the physical space corresponds to the vector $\mathbf{q}_1^{\perp} + \mathbf{q}_2^{\perp} + \mathbf{q}_2^{\perp}$ in the perpendicular space. Moreover, the modulus of the latter vector is minimal for the random combination of three basis vectors.

We show that algorithm (3) corresponds to the projection of sites of the four-dimensional cubic lattice that are located close to the physical space, thereby proving the equivalence of the proposed method and the projection method. For this, it is sufficient to show that the radius of the O_n geometric group in the perpendicular space $r_n^{\perp}$ (the maximal distance of the sites of the four-dimensional lattice to the physical space) is a finite quantity. As is clearly seen from Fig. 5, the validity of the equality

$$\mathbf{q}_1^{\perp} + \mathbf{q}_2^{\perp} + \mathbf{q}_3^{\perp} = -\left(\sqrt{2} - 1\right)\mathbf{q}_2^{\perp} = -\frac{1}{\delta_s}\,\mathbf{q}_2^{\perp} \tag{9}$$

directly follows from Eq. (5).

With Eqs. (6) and (9), it can be easily shown that the ultimate radii of the geometric groups $r_{n\to\infty}$ and $r_{n\to\infty}^{\perp}$ are

$$\begin{aligned} r_{n\to\infty} &= 1 + \sum_{n=2}^{\infty} \delta_s^{n-2} = \infty, \\ r_{n\to\infty}^{\perp} &= 1 + \sum_{n=2}^{\infty} \delta_s^{2-n} = 1 + \frac{1}{1-\delta_s^{-1}} = 2 + \frac{\sqrt{2}}{2}. \end{aligned} \tag{10}$$

Therefore, the distance of the sites of the four-dimensional lattice to the physical space does not exceed $2 + \sqrt{2}/2$. Hence, the proposed algorithm is quite valid.

3. MODELING THE RECIPROCAL OCTAGONAL LATTICE

We analyze the application of the proposed model to the reciprocal lattice of decagonal quasicrystals.

The square moduli of the respective vectors of physical, perpendicular, and four-dimension space, $\mathbf{Q}_{\square} = n_1\mathbf{q}_1 + n_2\mathbf{q}_2 + n_3\mathbf{q}_3 + n_4\mathbf{q}_4$, $\mathbf{Q}_{\perp} = n_1\mathbf{q}_1^{\perp} + n_2\mathbf{q}_2^{\perp} + n_3\mathbf{q}_3^{\perp} + n_4\mathbf{q}_4^{\perp}$, and $\mathbf{Q} = n_1\mathbf{u}_1 + n_2\mathbf{u}_2 + n_3\mathbf{u}_3 + n_4\mathbf{u}_4$, can be reduced to the form

$$\begin{aligned} |\mathbf{Q}_{\parallel}|^2 &= (n_1^2 + n_2^2 + n_3^2 + n_4^2) + \\ &\quad + (n_1n_2 + n_2n_3 + n_3n_4 - n_1n_4)\sqrt{2}, \\ |\mathbf{Q}_{\perp}|^2 &= (n_1^2 + n_2^2 + n_3^2 + n_4^2) - \\ &\quad - (n_1n_2 + n_2n_3 + n_3n_4 - n_1n_4)\sqrt{2}, \\ |\mathbf{Q}|^2 &= |\mathbf{Q}_{\parallel}|^2 + |\mathbf{Q}_{\perp}|^2 = 2(n_1^2 + n_2^2 + n_3^2 + n_4^2). \end{aligned} \tag{11}$$

Using the notations

$$\begin{aligned} N &= (n_1^2 + n_2^2 + n_3^2 + n_4^2) - \\ &\quad - (n_1n_2 + n_2n_3 + n_3n_4 - n_1n_4), \\ M &= n_1n_2 + n_2n_3 + n_3n_4 - n_1n_4, \end{aligned} \tag{12}$$

we can deduce that

$$|\mathbf{Q}_{\parallel}|^2 = N + M\delta_s, \tag{13}$$

which is similar to a relation existing for icosahedral quasicrystals (Cahn indexing [14]) and plain lattices of decagonal quasicrystals [15]:

$$|\mathbf{Q}_{\parallel}|^2 = N + M\tau. \tag{14}$$

Hence, the squared distance from the site of the four-dimensional lattice to the appropriate projection in the physical space is determined by the quantity $N\delta_s - M$:

$$|\mathbf{Q}_\perp|^2 = \frac{1}{\delta_s}(N\delta_s - M). \tag{15}$$

According to Refs. [5, 12, 13], the value of $|\mathbf{Q}_\perp|^2$ for the reciprocal lattice determines the intensity of diffraction reflections. It is worth noting that $|\mathbf{Q}_\perp|^2 \sim (N\tau - M)$ for icosahedral and decagonal lattices [14, 15].

Translation of the O_{n-1} geometric groups by $\delta_s^{n-2}\mathbf{q}_i$ corresponds, as follows from Eqs. (4) and (5), to shifting their centers to $(n_1n_2n_3n_4)$ sites of the (1110), (2320), (5750), (12 17 12 0), and $(K_n; K_n{+}K_{n-1}; K_n; 0)$ type. Substituting these indices in Eq. (11) yields the pairs of $N = K_n^2 + K_{n-1}^2$ and $M = 2(K_n^2 + K_nK_{n-1})$ values: (1, 2), (5, 12), (29, 70), (169, 408), ... Thus, the squared moduli of the geometric group shifting vectors can be expressed through the pairs of N and M numbers, which are, in fact, the neighboring elements of the Pell sequence. The corresponding number pairs satisfy the condition $M/N < \delta_s$, which is a necessary condition according to Eq. (15). It is possible to verify that the appropriate value of $|\mathbf{Q}_\perp|^2$ is rather small for these number pairs.

The overlapping of the O_4 geometric group on the electron diffraction pattern for an octagonal quasicrystal of the Mn_4(Al,Si) system is presented in Fig. 6*a*. Evidently, the sites of geometric groups totally coincide with the diffraction reflections. Nevertheless, there are some reflections of low intensities that have no counterparts among the sites of geometric groups (some of them are marked with arrows in Fig. 6). Substituting the group construction algorithm $O_2 = O_1 + \{\mathbf{q}_i\}O_1$ by $O_2 = O_1 + \{\sqrt{\mathbf{2}}\,\mathbf{q}_i\}O_1$, the algorithms for the successive groups being invariable, results in the occurrence of additional sites coinciding with the marked reflections (Fig. 6*b*). Hence, geometrically, the diffraction pattern is an octagonal quasicrystal of Mn_4 (Al,Si) related to the class of $O(\delta_s - 1, \delta_s^{n-2})$. Such a variation of the algorithm corresponds to extending the projection region in the four-dimensional space, because $r^\perp_{n\to\infty} = 2 + \sqrt{2}/2 + (\sqrt{2} - 1)$ in this case.

Table presents the characteristics of some reciprocal lattice sites located close to the origin. These sites have been generated according to algorithms (3),

$$O_2 = O_1 + \{\mathbf{q}_i\}O_1, \quad O_3 = O_2 + \{\sqrt{\mathbf{2}}\,\mathbf{q}_i\}O_2, \quad O_n = O_{n-1} + \{\delta_s^{n-3}\mathbf{q}_i\}O_{n-1}. \tag{16}$$

Multifold overlapping of sites arises as a result of the quasilattice construction using these algorithms. A number of such overlaps for different algorithms are presented in the last three columns of Table. Evidently, the correlation between the number of overlaps and the $|\mathbf{Q}_\perp|^2$ value similar to that inherent to the decagonal quasilattice [15] is observed for each of the listed algorithms.

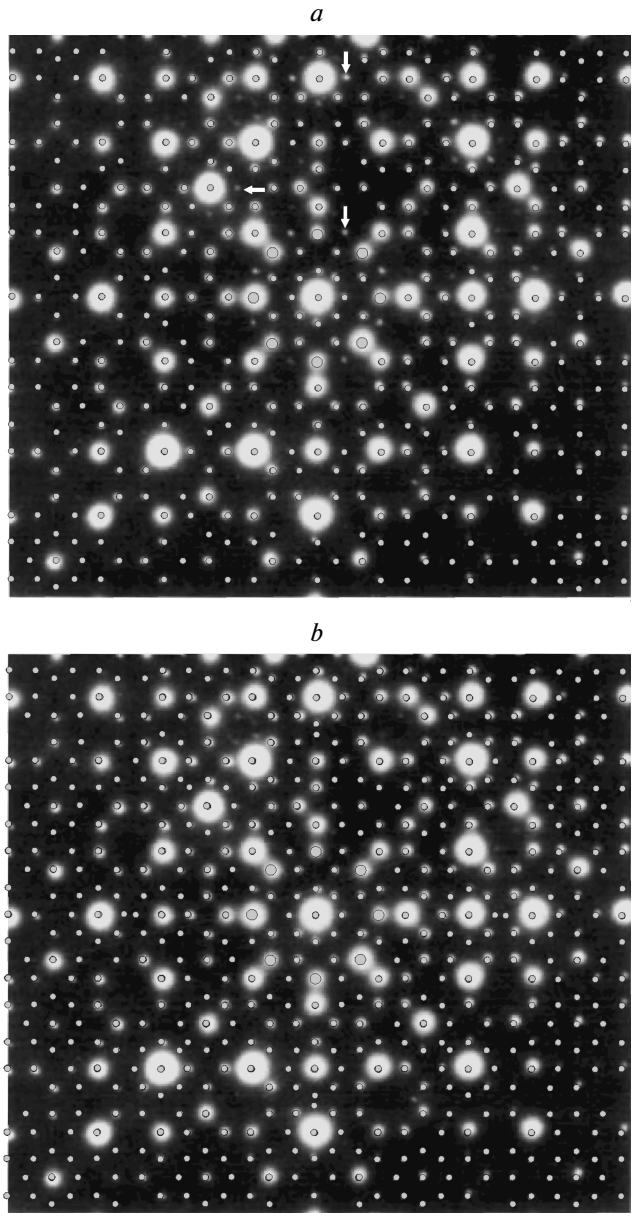

Fig. 6. Overlaps of the O_4 geometric group on the electron diffraction pattern for a quasicrystal of the Mn_4(Al,Si) system with the eightfold symmetry axis being oriented along the electron beam (the electron diffraction pattern is taken from Ref. [20])

Table. Characteristics of some sites of the O_7 groups constructed by the algorithms (3) and (16)

	$n_1n_2n_3n_4$	N	M	$\lvert\mathbf{Q}_\perp\rvert^2$	P (3)	P (16)
1	1–110	5	−2	5.828	5	78
2	–12–10	10	−4	11.657	–	11
3	001–1	3	−1	3.414	12	108
4	1000	1	0	1	43	223
5	11–11	6	−2	6.828	–	48
6	–111–2	11	−4	12.657	–	12
7	2–110	9	−3	10.243	–	22
8	02–10	7	−2	7.828	–	46
9	002–2	12	−4	13.657	–	6
10	1010	2	0	2	26	170
11	101–1	3	0	3	25	150
12	1100	1	1	0.586	48	224
13	2000	4	0	4	14	119
14	011–2	7	−1	7.414	–	54
15	2010	5	0	5	10	96
16	1110	1	2	0.172	73	257
17	2101	6	0	6	4	78
18	111–1	2	2	1.172	52	236
19	021–1	5	1	4.586	16	112
20	2100	3	2	2.172	28	162
21	112–1	5	2	4.172	15	110
22	2110	3	3	1.756	42	222
23	1210	2	4	0.343	78	286
24	22–10	7	2	6.172	–	61
25	121–1	3	4	1.343	44	196
26	2200	4	4	2.343	32	202
27	1300	7	3	5.757	8	96
28	2120	5	4	3.343	17	131
29	212–1	6	4	4.343	20	131
30	3110	7	4	5.343	5	81
31	122–1	5	5	2.929	32	192
32	2210	3	6	0.515	48	213
33	1310	5	6	2.515	27	151
34	221–1	3	7	0.101	104	332
35	131–1	6	6	3.515	32	172
36	2300	7	6	4.515	7	89
37	2220	4	8	0.686	54	276
38	312–1	9	6	6.515	3	63
39	222–1	5	8	1.686	36	185
40	3210	6	8	2.686	36	207

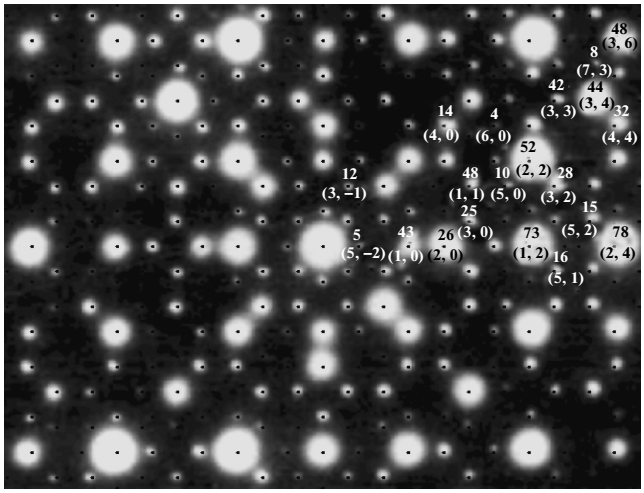

Fig. 7. (N, M) indices and the number of sites overlapping (the O_7 group, algorithm (3)) for the appropriate reflection in the electron diffraction pattern

Figure 7 presents $(N,\ M)$ indices and a number of sites overlaps (the O_7 group, algorithm (3)) for the appropriate reflection at the electron diffraction pattern for an octagonal quasicrystal of the $Mn_4(Al, Si)$ system. Evidently, a distinct correlation between the intensity of diffraction reflection and the number of overlaps is observed. This is in agreement with the data reported in Ref. [15].

Reasoning from the data in Table (by the number of overlaps and the $|\mathbf{Q}_\perp|^2$ value), the intensity $I_{(1,0)}$ should exceed $I_{(2,0)}$, and $I_{(1,2)} > I_{(2,4)}$, $I_{(1,1)} > I_{(1,0)}$, etc. This inconsistency with the experimental values of the intensities presented in Fig. 6 is thought to be caused by the fact that the values of intensities depend not only on the geometric factor determined by the $|\mathbf{Q}_\perp|^2$ value but also on the effects that are similar to the extinction effects in conventional fcc and bcc crystal lattices.

According to the obtained data, sufficiently high intensity should be inherent to the reflections characterized by the following combinations of (N, M) indices:

$$\begin{aligned}&(1,0);\,(2,0);\,(1,1);\,(1,2);\,(2,2);\\ &(3,3);\,(2,4);\,(3,4);\,(3,6);\,(3,7);\\ &(4,8);\,(5,8);\,(5,9);\,(6,10);\,(5,12);\ldots\end{aligned} \tag{17}$$

Reasoning from the three-dimensionality of the octagonal lattice and its periodicity along the eight-fold symmetry axis, the interplanar distances could be calculated by an equation similar to that obtained earlier for decagonal quasicrystals [15]:

$$\frac{1}{d^2} = \frac{N + M\delta_s}{a^2} + \frac{L^2}{c^2}. \qquad (18)$$

Here, a is a spacing parameter of a plain quasilattice and c is a spacing parameter along the eightfold symmetry axis.

In fact, in indexing the X-ray powder diffraction patterns, the L index does not exceed 2. Hence, the variety of the combinations of three (N, M, L) indices is rather limited. We note that in addition to the reflections of (N, M, L) type (with the N and M indices corresponding to values (17)), the reflections of the $(0, 0, L)$ type could also be observed at the diffraction pattern. Therefore, the indexing of the X-ray powder diffraction pattern for the octagonal quasicrystals is seen to be completely similar to that for the crystalline materials of the middle crystal systems.

4. CONCLUSIONS

The method of the quasicrystalline lattice modeling consisting in multiplication of the geometric groups was shown to be successfully used not only for decagonal but also for octagonal quasicrystals. The formal transition form the modeling of the decagonal quasicrystal lattice to the modeling of octagonal ones is realized by substituting the numerical parameter τ (the so-called "golden ratio") with the allied parameter δ_s ("silver ratio") and by changing of the source geometric group. The ascertained modification of the generic algorithm permits constructing different quasilattices of eight-fold symmetry.

The method for classifying different octagonal nodal structures, which obviously can be extended to quasicrystalline structure with different symmetries, has been proposed.

It was shown that using three (N, M, L) indices is quite sufficient to index the powder diffraction patterns for octagonal quasicrystals. The principal properties of (N, M) indices were proved to be completely the same as those for the decagonal quasilattice. In particular, the value of $(N\delta_s - M)$ provides information on the intensity of diffraction reflections. Thus, the proposed Cahn indexing [15] can be used not only for the icosahedral quasicrystals but also for the octagonal ones. The difference consists in adding an extra index.

Based on the experimental and theoretical data, the possible values of (N, M, L) indices corresponding to the diffraction reflections of sufficiently high intensity have been determined.

REFERENCES

1. S. E. Burkov, Phys. Rev. B **47**, 12325 (1993).
2. Yanfa Yan and S. J. Pennycook, Phys. Rev. B **61**, 14291 (2000).
3. V. V. Kovshevny, D. V. Olenev, and Yu. Kh. Vekilov, JETP **86**, 375 (1998).
4. Ю. Х. Векилов, Е. И. Исаев, Кристаллография **52**, 6 (2005).
5. W. Steurer and S. Deloudi, *Crystallography of Quasicrystals: Concepts, Methods, and Structures, Springer Series in Materials Sciences* 126, Springer (2009), p. 384.
6. R. Ammann, B. Grunbaum, and G. C. Shephard, Discrete Comput. Geom. **8**, 1 (1992).
7. F. P. N. Beenker, *Algebraic Theory of Non-Periodic Tilings of the Plane by Two Simple Building Blocks: a Square and a Rhombus*, TH-Report 82-WSK04 (1982).
8. P. J. Lu, K. Deffeyes, P. J. Steinhardt, and N. Yao, Phys. Rev. Lett. **87**, 275507 (2001).
9. V. E. Dmitrienko, V. A. Chizhikov, S. B. Astaf'ev, and M. Kleman, Crystallogr. Rep. **49**, 547 (2004).
10. A. Singh and S. Ranganathan, J. Mater. Res. **14**, 11 (1999).
11. S. Ranganathan, E. A. Lord, N. K. Mukhopadhyay et al., Acta Crystallogr. Sect. A **63**, 1 (2007).
12. Y. K. Vekilov and M. A. Chernikov, Phys. Usp. **53**, 537 (2010).
13. C. Janot, *Quasicrystals: A. Primer*, 2nd ed., Oxford University Press, New York (1994), p. 409.
14. J. W. Cahn, D. Shechtman, and D. Gratias, J. Mater. Res. **1**, 13 (1986).
15. V. V. Girzhon, V. M. Kovalyova, O. V. Smolyakov et al., J. Non-Crystall. Sol. **358**, 137 (2012).
16. J.-M. Dubois, *Useful Quasicrystals*, World Scientific, Singapore–London (2005), p. 481.
17. M. Bicknell, Fibonacci Quart. **13**, 345 (1975).
18. Y. Roichman and D. G. Grier, arXiv:cond-mat/0506283.
19. D. Levine and P. Steinhardt, J. Phys. Rev. Lett. **53**, 26 (1984).
20. K. H. Kuo, J. Non-Crystall Sol. **117/118**, 754 (1990).