# CRYSTALLOGRAPHY OF DODECAGONAL QUASICRYSTALS

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**Abstract.** A detailed model structure of dodecagonal quasicrystals is proposed which applies to both dodecagonal Ni-Cr and V-Ni or V-Si-Ni. This model structure can be represented as the restriction of a 5d periodic structure to a 3d subspace, which is identified with physical space. The point group and the space group of the 5d periodic structure are determined. The latter is non-symmorphic, containing a set of glide "planes" and a screw axis. These space group elements lead to characteristic extinctions in the Fourier spectrum, which should be experimentally observable. A numeric calculation, which includes multiple scattering effects for electron diffraction, confirms the presence of the extinctions predicted by the space group analysis. The model structure proposed here serves as a very instructive example how crystallographic concepts, such as Bravais type, point group, or space group, can be applied to quasicrystals.

## 1. INTRODUCTION

The detailed atomic structure of quasicrystals is to a large extent still an unsolved problem. Here we present such a model structure with detailed atomic positions for the case of dodecagonal quasicrystals[1-3]. Dodecagonal quasicrystals have first been observed by Ishimasa, Nissen and Fukano[1,2] in small particles of Ni-Cr produced by the so-called gas evaporation technique. Under electron diffraction, this new phase produces a crystallographically forbidden twelvefold symmetric diffraction pattern. The dodecagonal phase always coexists with the crystallographic $\sigma$-phase, to which it must be closely related. This can be deduced from the fact that the corresponding high resolution electron micrographs (HREMs) look very similar. This will enable us to derive a model structure for the dodecagonal phase directly from the structure of the $\sigma$-phase. More recently, the same phase had also been observed in V-Ni and V-Si-Ni alloys by Chen et al.[3]. Their specimens are prepared by the conventional piston-and-anvil technique. This allows

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in particular to observe also diffraction patterns with incoming beam perpendicular to the twelvefold axis. These diffraction patterns show that the dodecagonal phase is periodic along the z-axis. In the case of the small particles of Ni-Cr it was not possible to take such pictures because of the multi-phase character of the particles.

The close resemblance of the HREMs of the dodecagonal and the $\sigma$-phase will be the starting point in the derivation of a model structure of the dodecagonal phase. These HREMs[1-3] show bright spots which form the vertices of a tiling. In the case of the $\sigma$-phase, the tiling is the (periodic) semi-regular tesselation with Schläfli symbol $(3^2 \cdot 4 \cdot 3 \cdot 4)$, consisting of equilateral triangles and squares only. In the dodecagonal case however, the tiling consists of the same triangles and squares, together with some additional 30°-rhombuses. Moreover, the local configurations in the dodecagonal tiling look very similar to those of the $\sigma$-phase tiling. Therefore, it is very tempting to identify the triangles and squares in the dodecagonal tiling with the corresponding building blocks of the $\sigma$-phase, which are triangular and square prisms respectively. Since the 30°-rhombus is rather thin, its decoration is then also fixed whenever it is isolated, which is practically always the case. Following the tiling, with these three building blocks we can then construct a layer which we stack periodically to obtain a model structure for dodecagonal quasicrystals.

In a first step, with the help of the projection method we construct quasiperiodic tilings with dodecagonal symmetry. This is achieved by projecting from the 4d dodecagonal lattice[4] with a suitably constructed acceptance domain. This projection method provides us with an analytical description of one layer of the model structure. We will be concerned mainly with one of these tilings, which resembles as closely as possible the experimentally observed HREMs. More details about other tilings which might be relevant for dodecagonal quasicrystals will be published elsewhere[5]. In a next step, we construct a 5d periodic structure such that the restriction of this periodic structure to a suitably embedded 3d subspace (physical space) yields the desired model structure. The Fourier spectrum of the model structure is then the projection to 3d physical reciprocal space of the Fourier spectrum of the 5d periodic structure.

The construction of the 5d periodic structure makes manifest that it is invariant under a certain non-symmorphic space group, which is one of the 132 space groups for quasicrystals[6] which can be obtained from 5d periodic structures. In fact, this space group contains a screw axis and a set of glide "planes". These symmetry elements lead to characteristic extinctions in the Fourier spectrum, which should be experimentally observable. Finally, we calculate electron diffraction patterns of the model structure for various directions of the incoming beam, and compare them to the experimentally observed ones, as far as they are available. It turns out that it is not sufficient to just calculate the Fourier transform of the model structure, which would lead to a very poor fit. Rather, since electrons are scattered very strongly by the coulomb potential, we have to include multiple scattering effects. Including these effects, we obtain a very nice fit with the experimental results. Moreover, we can verify that the characteristic extinctions derived in the space group analysis are actually present in the calculated diffraction patterns. Unfortunately, the corresponding experimental pictures are still missing.

## 2. DODECAGONAL TILINGS

In this section we derive quasiperiodic dodecagonal tilings suitable for decoration with the basic building blocks of the $\sigma$-phase. Quasiperiodic tilings with a given symmetry are usually obtained by projection from a higher dimensional lattice with this symmetry. Here we therefore have to construct a suitable lattice $L$ with twelvefold symmetry. For the sake of simplicity, we are interested only in lattices of minimal dimension. A further requirement is that the twelvefold symmetry operation $A$ leaving $L$ invariant has a 2d invariant subspace $E^{\parallel}$ on which it acts with the usual 2d representation

$$r_{\parallel}(A) = \begin{pmatrix} \cos(\pi/6) & -\sin(\pi/6) \\ \sin(\pi/6) & \cos(\pi/6) \end{pmatrix}. \tag{1}$$

In a first step, we determine the representation (and its dimension) with which $A$ acts on $L$. As is well known, a 2d lattice cannot have twelvefold symmetry. If such a lattice would exist, we could express the representation matrices of its point group with respect to a lattice basis. In such a basis, these representation matrices would then have only integer entries, and in particular integer traces. The traces however are the same in every basis, and since $tr(r_{\parallel}(A)) = 2\cos(\pi/6)$ is not an integer, such a lattice cannot exist. Above reasoning suggests however a way to solve this problem: we simply have to add more irreducible representation of $C_{12}$ to $r_{\parallel}$ such that the total trace becomes an integer. As it turns out, it is sufficient to add one more irreducible representation: there is a unique (up to equivalence) 2d irreducible representation $r_{\perp}$ acting on an invariant subspace $E^{\perp}$, whose trace combines with the trace of $r_{\parallel}$ to an integer, namely

$$r_{\perp}(A) = \begin{pmatrix} \cos(5\pi/6) & -\sin(5\pi/6) \\ \sin(5\pi/6) & \cos(5\pi/6) \end{pmatrix}. \tag{2}$$

Therefore, $r = r_{\parallel} \oplus r_{\perp}$ is a good candidate for the representation with which $A$ acts on $L$. Let $\mathbf{e}_1$ be a vector in a basis of $L$. Clearly, $\mathbf{e}_1$ must have components in both $E^{\parallel}$ and $E^{\perp}$. If we act repeatedly with $r(A)$ on $\mathbf{e}_1$, we obtain a star of twelve vectors $\{\mathbf{e}_1, \ldots, \mathbf{e}_{12}\}$, whose projections on $E^{\parallel}$ and $E^{\perp}$ can be expressed in a suitable orthonormal basis as

$$\begin{aligned} \mathbf{e}_i^{\parallel} &= a_{\parallel}(\cos((i-1)\pi/6), \sin((i-1)\pi/6)) \\ \mathbf{e}_i^{\perp} &= a_{\perp}(\cos(5(i-1)\pi/6), \sin(5(i-1)\pi/6)). \end{aligned} \tag{3}$$

Note that only four of these twelve vectors are rationally independent. The point is that the vectors in any orbit of a subgroup of $C_{12}$ add up to zero. For instance, the subgroup of order two has six different orbits and generates the relations $\mathbf{e}_{i+6} = -\mathbf{e}_i$. The subgroup of order three has four orbits and generates therefore four relations, two of which are rationally independent, namely $\mathbf{e}_5 = \mathbf{e}_3 - \mathbf{e}_1$ and $\mathbf{e}_6 = \mathbf{e}_4 - \mathbf{e}_2$. These relations allow us to express all twelve vectors as integer linear combinations of $\{\mathbf{e}_1, \ldots, \mathbf{e}_4\}$. Therefore, the Z-span of these four vectors, which we will use as a basis in the following, is indeed a four dimensional lattice invariant under the representation $r$ of $C_{12}$.

If we compare these lattices parametrized by $a_\parallel$ and $a_\perp$ to the complete classification of crystallographic groups in four dimensions[4], we see that these lattices form the so called dodecagonal Bravais class in four dimensions. The point group of these lattices is $D_{24}$, the dihedral group of order 24, generated by

$$A = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \tag{4}$$

where we have expressed the twelvefold rotation $A$ and the mirror $B$ with respect to the lattice basis $\{\mathbf{e}_1, \ldots, \mathbf{e}_4\}$. Note that there are no other four dimensional dodecagonal lattices. However, for special ratios of the parameters $a_\parallel$ and $a_\perp$ we obtain lattices with even larger symmetry. Since the additional symmetry elements do not leave the spaces $E^\parallel$ and $E^\perp$ seperately invariant however, these symmetries are not interesting for quasicrystals.

The vertices of quasiperiodic tilings are usually obtained by projecting the lattice points of $L$ onto $E^\parallel$ which are contained in a strip $S = C \times E$, where the acceptance domain $C$ is some subset of $E^\perp$, and $E$ is a plane parallel to $E^\parallel$. The size and shape of $C$ determines the local configurations of the tiling. Recall that we are interested in constructing tilings consisting of eqilateral triangles, squares and a few isolated 30°-rhombuses, all of edge length $a_\parallel$. The lattice parameter $a_\perp$ is arbitrary. If a certain local configuration should (not) occur in the tiling, we have to take care that the projections of the corresponding lattice points onto $E^\perp$ do (not) fit simultaneously into $C$. If we want to avoid adjacent rhombuses, we have to choose $C$ so small that $\mathbf{x}_\perp$, $\mathbf{x}_\perp + \mathbf{e}_1^\perp$, $\mathbf{x}_\perp + \mathbf{e}_2^\perp$ and $\mathbf{x}_\perp + \mathbf{e}_3^\perp$ (or a symmetry equivalent set) do not fit simultaneously into $C$ for any choice of $\mathbf{x}_\perp$. The largest such acceptance region $C_a$ which is connected is shown in Fig. 1. This acceptance region is non-convex, with a small diameter of $2a_\perp$, and a large diameter of $4\cos(\pi/12)a_\perp/\sqrt{3}$. A tiling constructed with this acceptance region is shown in Fig. 2. It consists indeed of the desired tiling units and looks remarkably similar to the HREMs[1-3]. An even better coincidence can be obtained by rearranging locally some of the tiles. This is known as Hendricks-Teller disorder[7,8], which is very common in quasicrystals. If we wanted to eliminate all rhombuses, we had to choose an even smaller acceptance region $C_b$ (Fig. 1), which leads to the tiling shown in Fig. 3. In this tiling, the 30°-rhombuses have been replaced by a new tiling unit, an asymmetric hexagon. If we choose as acceptance region the convex hull $C_c$ of $C_a$

(Fig. 1) we obtain a tiling first constructed by Stampfli[9] by means of a grid[10]. This tiling is shown in Fig. 4. It should be noted that these tilings have been discussed also by Niizeki and Mitani[11]. Henceforth, we will concentrate on the tiling of Fig. 2, without Hendricks-Teller disorder.

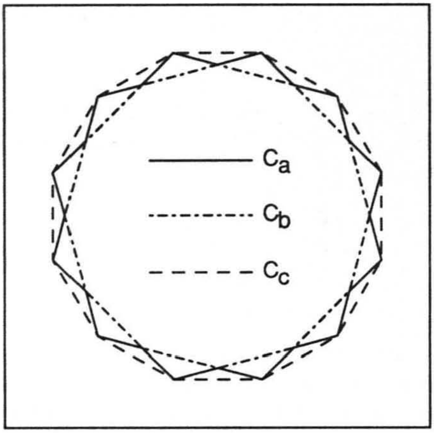


Fig. 1: Various acceptance regions

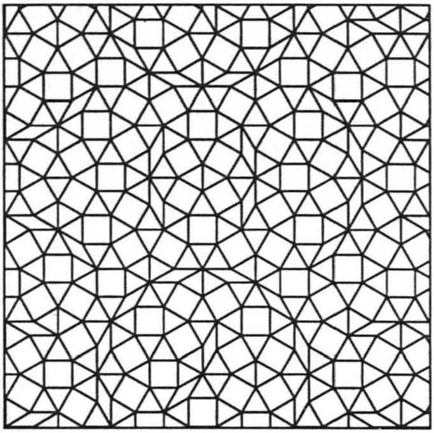

Fig. 2: Tiling with acceptance region $C_a$

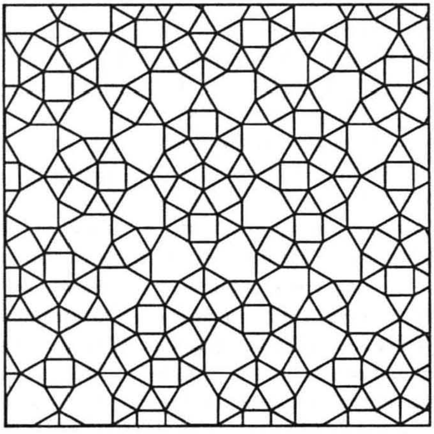

Fig. 3: Tiling with acceptance region $C_b$

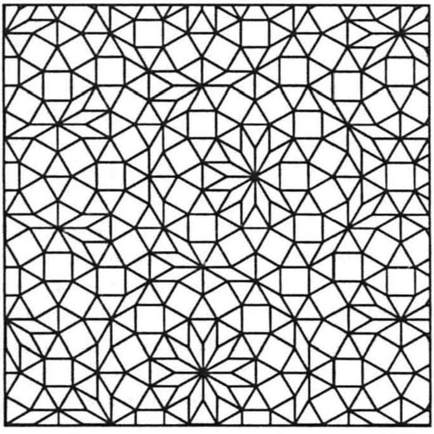

Fig. 4: Tiling with acceptance region $C_c$

## 3. THE ATOMIC STRUCTURE

Next we decorate the squares and triangles of the dodecagonal tiling with the structural units of the $\sigma$-phase. These units are shown in Fig. 5, where dotted circles represent atoms* at $z = 1/4$ and $z = 3/4$, open circles atoms at $z = 0$ and full circles atoms at $z = 1/2$ (in units of the periodicity in z-direction). From Fig. 5 one can also see that the decoration of the (isolated) rhombuses is forced by that of the squares and triangles. This decoration has already been proposed in Ref. 1. From Fig. 5 we see that the layers at $z = 1/4$, $z = 3/4$ contain atoms at the vertices of the dodecagonal tiling, whereas the layers at $z = 0$ and $z = 1/2$ consist of atoms placed on the midpoints of some bonds, along with possibly some atoms in the interior of the squares and triangles, depending on the orientation of these figures (see Fig. 5). In the $z = 0$ layer, only bonds parallel to $\mathbf{e}_i^{\parallel}$ with $i$ even are occupied, whereas in the $z = 1/2$ layer those with $i$ odd are occupied, so that the decoration of the latter two layers breaks the dodecagonal symmetry of the underlying tiling to a hexagonal one. Therefore, if we denote the $z = 1/4$ (or $z = 3/4$) layer by $A$, the $z = 0$ layer by $B$ and the $z = 1/2$ layer by $C$, the structure is given by a stacking $\ldots ABAC \ldots$, where the layers $A$ have dodecagonal symmetry, and the layers $B$ and $C$ have hexagonal symmetry.

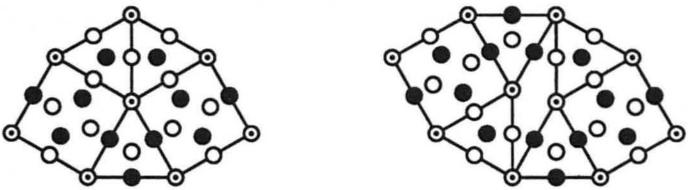

Fig 5: Typical configurations in the $\sigma$-phase (left) and the quasicrystal (right). For description see text.

A similar structure for dodecagonal quasicrystals has been proposed by Yang and Wei[12]. Their structure can be understood as an alternating stacking of a layer $D$ and its mirror image $\tilde{D}$ (where the mirror plane is perpendicular to the z-axis). The layer $D$ is essentially a decoration of the vertices of the tiling of Fig. 3 by slightly distorted hexagonal antiprisms containing an additional atom at their center. Because of the great similarity of this structure to ours, the diffraction pattern is expected to be very similar too. Nevertheless we consider our decoration as preferable, for the following reason. As we have argued above, the bright spots in the HREMs[1-3] can be identified with those columns of atoms containig the atoms of the layers $A$. These columns are doubly occupied as compared to those containing the atoms of the layers $B$ or $C$. Now in these HREMs most of the asymmetric hexagons, as they occur in Fig. 3, contain an additional bright spot in their interior, which suggests a disection of these hexagons into a square, two equilateral triangles and a thin rhomb. Therefore, our decoration, which breaks

*we do not know which kind of atom occupies what kind of position the threefold symmetry of these hexagons, seems more appropriate than that of Yang and Wei.

## 4. THE 5D PERIODIC STRUCTURE

Despite of the presence of the hexagonal layers $B$ and $C$ the structure has point group 12/mmm and therefore twelvefold symmetric Fourier spectrum. Since the main axis of the hexagonal layers are turned with respect to each other by 30°, the stacking sequence suggests a $12_6$-screw axis. Moreover, the mirror $B$ (4) maps the main axis of the layer $B$ onto those of the layer $C$, and vice versa, so that we can expect as well that the mirror $B$ is actually a glide mirror, translating the structure by half a period length into z-direction.

To make these intuitive arguments about the space group more rigorous, we construct a 5d periodic structure with this space group such that the quasiperiodic structure described above is the restriction of this periodic structure to a suitably embedded 3d subspace.

In a first step, we have to reformulate the projection method. Instead of projecting all vertices in the strip $L \cap (C \times E)$ onto $E^{\parallel}$ and then decorating them with the scattering density $\rho(\mathbf{x}_{\parallel})$ of an atom or cluster of atoms, we can as well decorate each vertex of $L$ with a density $\rho(\mathbf{x}_{\parallel}) \cdot \chi_{\bar{C}}(\mathbf{x}_{\perp})$ (where $\bar{C}$ is the set $C$ inverted at the origin, and $\chi_{\bar{C}}(\mathbf{x}_{\perp})$ the characteristic function of $\bar{C}$) and then take the intersection of the so obtained periodic density with $E$, which yields the same result. This latter formulation, first used by Janssen[13)] and Bak[14)], is much more flexible than the original projection method. In particular, it is easy to add more atoms of various types at different positions in the unit cell of $L$, each with its own characteristic acceptance region. In this way also very complicated quasicrystals (including atomic decoration) can be viewed as the restriction of a higherdimensional periodic structure to physical space. Since the Fourier spectrum of such an restriction is just the projection of the Fourier spectrum of the higherdimensional periodic structure to physical space, classical crystallography can be applied to the periodic structure to determine the Bravais class, point symmetry and space group associated with a quasicrystal. The quasicrystal inherits in this way the point symmetry and the characteristic extinctions associated with the higherdimensional space group. Therefore, we can speak of the space group of a quasicrystal, which we define to be that of the associated higherdimensional periodic structure.

Next we construct the 5d periodic structure. There is only one dodecagonal lattice in five dimensions[15)], $L^5 = L \times a_z Z$, where $a_z$ is the periodicity in z-direction. This lattice is contained in a 5d space $E^{\parallel} \oplus E^{\perp} \oplus E_z$. It is interesting to note that $L^5$ cannot have any centerings, i.e. all layers $z = const.$ are the same. Suppose for the moment that this is not so. Then, any lattice vector $\mathbf{x}$ with smallest possible non-zero component $x_z$ in z-direction is not parallel to the z-axis. Let us now act with the subgroups $C_2$ and $C_3$ of $C_{12}$ on $\mathbf{x}$. If we add up the vectors in the orbits of these subgroups, we obtain vectors of length $2x_z$ and $3x_z$ which are parallel to the z-axis. Since their difference has length $x_z$ and is also parallel to the z-axis, we arrive at a contradiction, which proves our hypothesis to be false. Therefore, we have to consider only the lattice $L^5$. In the following, we will always use the lattice basis $\{\mathbf{e}_1, \ldots, \mathbf{e}_4, \mathbf{e}_z\}$, where $\mathbf{e}_z$ is a basis vector in z-direction. Sometimes, it is conveniant to use the compound notation $(\mathbf{x}, z)$, where the first item denotes the first four coordinates in $E^{\parallel} \oplus E^{\perp}$. We construct the periodic structure in such a way that it becomes manifestly invariant under the space group generated by $(A, a)$, $(B, b)$, $(-I, 0)$ and the set of lattice translations. Here, $A$ and $B$ are the generators (4), $(X, x)$ denotes the Euclidean transformation $\mathbf{y} \rightarrow X\mathbf{y} + x$, and $a = b = (0, 0, 0, 0, \frac{1}{2})$.

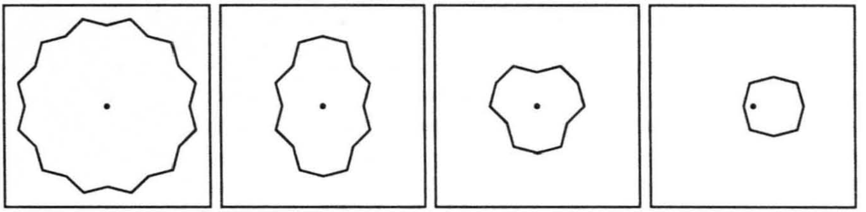

Fig. 6: Acceptance regions for atoms on a vertex, on a bond, in a triangle and in a square (from left to right).

First we place an atom with acceptance region $C_a$ (see Fig. 6) at $(\mathbf{v}, \frac{1}{4})$, where $\mathbf{v}$ is a lattice site of $L$. Then we act with all the desired symmetry elements on this motif. The lattice translations put an atom at all sites in $L^5 + (0, \frac{1}{4})$. Moreover, for each atom at $(\mathbf{v}, z)$ the screw axis puts another copy at $(\mathbf{v}, z + \frac{1}{2})$. Since the acceptance region has dodecagonal symmetry, it is not changed under this screw operation. The other symmetry elements leave the structure obtained so far invariant. Note that the acceptance region is invariant also under the mirror $B$. Next we insert the atoms on the bonds of the tiling. We put an atom on the midpoint of a bond of $L$ which is parallel to $\mathbf{e}_2$, at $z = 0$. The acceptance region is chosen in such a way that it intersects physical space $E \times E_z$ if and only if the acceptance regions of the two atoms at the vertices at the ends of this bond intersect $E \times E_z$ too. This results in an asymmetric acceptance region shown in Fig 6. Then we add all translation equivalent atoms. Appling the screw operation puts atoms on all the other bonds, those on bonds parallel to $\mathbf{e}_i$ with $i$ even at $z = 0$, the remaining ones at $z = \frac{1}{2}$. Due to the rotational part of the screw operation, the acceptance regions of all these atoms will have their proper orientation. Again, the glide mirror $(B, b)$ leaves the structure obtained so far invariant. Analogously, we put an atom in the middle of a triangle in the lattice $L$ which projects to a triangle of the tiling, at $z = 0$ or $z = \frac{1}{2}$ (depending on the orientation of this triangle), and with acceptance region shown in Fig. 6. This acceptance region intersects physical space if and only if those at the corners of the triangle do this too. Acting then with the space group on this atom puts copies to the interiors of all triangles at the correct z coordinate, depending on the orientation of these triangles. Finally, we put an atom into the interior of a square in the lattice $L$. This time, we have to use an acceptance region which is not centro-symmetric (Fig 6), because the four corners of the square, whose acceptance regions have to cut physical space too, are at different distances. Acting then with the space group on this atom completes the structure. Note that the space group takes care that all atoms have their correct $z$-value, and that their acceptance regions have the proper orientation. Therefore, the 5d periodic structure is manifestly invariant under a non-symmorphic space group, and the quasicrystal structure is the restriction of this periodic structure to physical space $E \times E_z$.

## 5. THE RECIPROCAL LATTICE AND EXTINCTION RULES

First, we calculate the reciprocal lattice $\hat{L}^5$ of $L^5$. Since $L^5$ is a periodic stacking of $L$, $\hat{L}^5$ is given by $\hat{L} \oplus (2\pi/a_z)Z$, so that is sufficient to calculate the reciprocal lattice $\hat{L}$ of $L$. It is conveniant to choose $a_\perp = a_\parallel$, but any other choice of $a_\perp$ would give the same result. The metric tensor of $L$, defined by $g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j$, is given by

$$g = a_\parallel^2 \begin{pmatrix} 2 & 0 & 1 & 0 \\ 0 & 2 & 0 & 1 \\ 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 2 \end{pmatrix}. \tag{5}$$

Let $\{\mathbf{b}_i\}$ be the basis reciprocal to $\{\mathbf{e}_i\}$, i. e. $\mathbf{b}_i \cdot \mathbf{e}_j = 2\pi\delta_{ij}$. Then, if the $i^{th}$ row of the matrix $b$ contains the components of $\mathbf{b}_i$ with respect to the basis $\{\mathbf{e}_i\}$, we have that

$$(bg)_{ij} = \sum_k b_{ik}\mathbf{e}_k \cdot \mathbf{e}_j = \mathbf{b}_i \cdot \mathbf{e}_j = 2\pi\delta_{ij}, \tag{6}$$

i. e. $b$ is equal to $2\pi$ times the matrix inverse of $g$, which is given by

$$g^{-1} = \frac{1}{3a_\parallel^2} \begin{pmatrix} 2 & 0 & -1 & 0 \\ 0 & 2 & 0 & -1 \\ -1 & 0 & 2 & 0 \\ 0 & -1 & 0 & 2 \end{pmatrix}. \tag{7}$$

Comparison with (3) shows that $\hat{L}$ is again a dodecagonal lattice, but this time with lattice parameters

$$\hat{a}_\parallel = \frac{2\pi}{3a_\parallel^2} \cdot a_\parallel\sqrt{3} = \frac{2\pi}{a_\parallel\sqrt{3}}, \quad \hat{a}_\perp = \frac{2\pi}{a_\perp\sqrt{3}}. \tag{8}$$

Therefore, the peak positions in the quasiperiodic plane are generated by a twelve-fold symmetric star of vectors $\mathbf{b}_i^\parallel$ which have length $\hat{a}_\parallel = 2\pi/a_\parallel\sqrt{3}$.

Let us now turn to the extinctions in the Fourier spectrum caused by the space group. Suppose a periodic structure $\rho(r)$ is invariant under a Euclidean transformation $(X, x)$, i.e. $\rho(r) = \rho(Xr + x)$. Then, the Fourier transform of $\rho$ satisfies $\hat{\rho}(k) = e^{ik\cdot x}\hat{\rho}(X^{-1}k)$. Now, if for a given $k$

$$e^{ik\cdot x} \neq 1 \quad \text{and} \quad \hat{\rho}(k) = \hat{\rho}(X^{-1}k), \tag{9}$$

then $\hat{\rho}(k)$ must necessarily vanish. When (9) holds it is even always possible to find a $k$ such that $X^{-1}k = k$ and $e^{ik\cdot x} \neq 1$.

In the present case this means that due to the screw symmetry of dodecagonal quasicrystals we can expect that all peaks $(\mathbf{k}, k_z)$ are extinct whenever $k_z$ is odd. Similarly, the glide mirror symmetry causes all peaks $k$ contained in a glide plane and with $k_z$ odd to be absent. These extinctions can be understood also intuitively. The point is that at least in kinematical theory scattering with a scattering vector $q$ is sensitive only to the projection of the structure onto this scattering vector. But since the projection of the layers $B$ and $C$ onto the z-axis give the same density, a scattering vector parallel to the z-axis sees a structure with half the period length, and therefore every second peak is absent. Similarly one can argue for the glide mirror plane, though the situation is slightly more complicated there.

One should note however that multiple diffraction, which occurs always with electron diffraction, might distroy this effect. Nevertheless, such extinctions are very typical for quasicrystals periodic in one direction. They have been observed already for decagonal[16] and octagonal[17] quasicrystals. Our numeric calculations (see next chapter), which include multiple scattering, show that these extinctions have to be expected also in the dodecagonal case.

## 6. CALCULATION OF THE DIFFRACTION PATTERN

Since we have described our quasicrystal structure by means of a 5d periodic structure, it is now easy to compute its Fourier spectrum. We simply have to calculate the Fourier transform of the periodic structure and then project it onto physical reciprocal space. The Fourier transform of a periodic structure is obtained by first calculating the Fourier transform of the contents of a unit cell and then convoluting it with the reciprocal lattice, just as one does it with 3d crystals. The $z = 0$ layer of the Fourier transform of the quasicrystal is shown in Fig. 7. The radius of the circles is proportional to the *amplitude* (not intensity) of a peak. We see that Fig. 7 consists essentially of a single ring of very strong spots, the next weaker ones being more than ten times weaker (in intensity). This is very different from what one sees in electron diffraction[1−3], and also different from what one obtaines if one puts just atoms at the vertices of the tiling[11], which would actually give a very good fit with experiment. The additional hexagonal layers lead to destructive interferences, so that only a few very prominent peak survive.

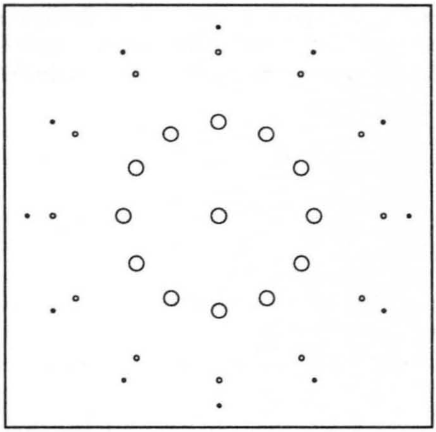

Fig. 7: The Fourier transform

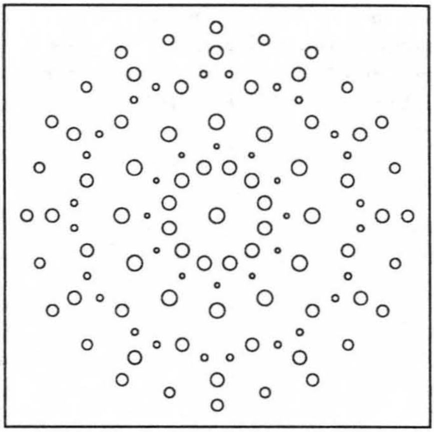

Fig. 8: Dodecagonal diffraction pattern

We have to recall however that electrons are very strongly scattered by the coulomb potential, so that we have to take into account multiple scattering effects. This can be done by Darwin's method[18]. In electron diffraction, the incoming k-vector is much larger than the relevant scattering vectors, so that all q-vectors which contribute to elastic scattering are contained essentially in tangent plane of Ewald's sphere, i.e. only scattering vectors contribute which are contained in a plane through the origin and perpendicular to the incoming $k$-vector. All scattered beams can be indexed by the reciprocal vectors in this plane. Let $\phi_q$ denote the amplitude of such a scattered beam, and $f_q$ the amplitude of the Fourier transform. While the beams pass through the quasicrystal, their amplitudes develop according to[18]

$$\frac{d\phi_k}{dz} = \lambda i \sum_q \phi_{k-q} f_q, \tag{10}$$

where $z$ measures the depth in the quasicrystal in the incoming beam direction, and $\lambda$ is a constant depending on the density and type of atoms in the material. The sum extends over all reciprocal vectors in the plane perpendicular to the incoming beam, and the factor $i$ in front of the sum ensures that the total intensity remains constant. In fact, it is easy to show that

$$\frac{d}{dz} \sum_q \phi_q \phi_q^* = 0. \tag{11}$$

Starting with $\phi_0 = 1$, $\phi_q = 0$ $(q \neq 0)$ equation (10) can easily be integrated numerically. We have chosen the integration domain such that we obtain best possible coincidence with the experimentally observed patterns. The step width in the numerical integration was determined such that about 40 iterations were necessary. In the dodecagonal plane, 3721 scattering vectors were included, whereas in the planes containing the z-axis 729 vectors were sufficient. The results are shown in Fig. 8 (dodecagonal plane) and Figs. 9 and 10 (mirror plane* and glide mirror plane respectively). Again, the radii of the circles are proportional to the amplitudes.

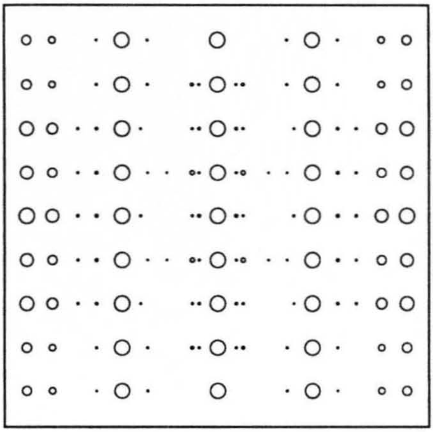

Fig. 9: Diffraction pattern in mirror plane

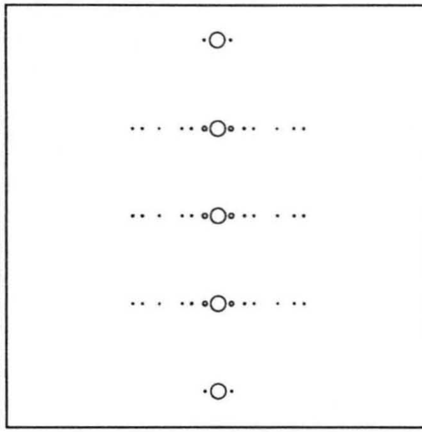

Fig. 10: Diffraction pattern in glide plane

All these calculated diffraction patterns compare very well to the observed ones, as far as available[1–3]. If we compare Figs. 7 and 8 we see that due to multiple scattering many additional peaks have appeared, in particular two additional rings very close to the center. This is very similar to what happens in the $\sigma$-phase of Fe-Cr. The $\sigma$-phase has peaks very close these peaks of the dodecagonal phase. Calculations of T. Ishimasa (private communication) show that for very thin samples of the $\sigma$-phase, the peaks corresponding to the two inner rings are very weak, those near the positions of the very strong peaks of Fig. 7 are very strong. When the thickness of the sample increases, the weak peaks become much stronger however, whereas the strong peaks get weaker, until the three classes of peaks are of about the same intensity. The dependence of these intensities on sample thickness suggests that that this effect is due to multiple scattering. This analogy with the $\sigma$-phase supports our hypothesis that multiple scattering is very important also in the dodecagonal case.

In Fig. 10 we see that the predicted extinctions are indeed present (i.e. the corresponding peaks are absent). Only in Fig. 9 the forbidden odd peaks on the z-axis are not extinct due to multiple scattering effects. This effect can be observed also in decagonal and octagonal quasicrystals[16,17]. Interesting to note is also that the layers in Fig. 10 which are still present are very weak. The reason

*the planes between two neighboring glide planes are true mirror planes is that in the corresponding plane there is none of the very strong peaks of Fig. 7, and the intensity remains essentially on the z-axis. May be it will be difficult to observe such a diffraction pattern, and this might be the reason why in Ref. 3 no such pattern is published, although it would of course be very interesting because of the extinctions.

## 7. CONCLUSIONS

In conclusion, we have presented a detailed model structure for dodecagonal quasicrystals, whose calculated diffraction patterns are in good agreement with the experimentally observed ones. As we have seen, it is absolutely essential to take multiple diffraction effects into account, without which the experimental diffraction patterns cannot be explained. The proposed model structure is the restriction of a 5d periodic structure to 3d physical space. This 5d structure has a non-symmorphic space group, which has direct consequences for the quasicrystal. This model structure therefore naturally illustrates how crystallographic concepts can be applied to quasicrystals: *quasicrystallography* is simply the crystallography of the associated higherdimensional periodic structures.

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