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Indexing of Electron Diffraction Patterns of Icosahedral and Decagonal Phases

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1. Introduction

The atomic arrangements of solids fall into two broad categories. First refers to long range translational order giving rise to sharp diffraction patterns. Second relates to an atomic order that displays diffuse halos. Prior to the discovery of Quasiperiodic translational order in rapidly solidified Al-Mn alloys [1], sharp diffraction peaks were considered to be synonymous to possession of periodic translational orders in solids. The electron diffraction patterns reported in reference [1] were found to be invariant under icosahedral point group ($m\bar{3}5$) symmetry. Any elementary text on crystallography begins by showing that 5-fold symmetry is incompatible with periodic lattice translations. Thus, it was proved beyond doubt that Shetchman et al.[1] have discovered a new state of order in solids. Readers may go through the notes given in annexure **A** for the excitement and importance of this discovery. The underlying atomic arrangement [1] was believed to possess “Quasiperiodic” translational order and due to invariance of diffraction patterns under icosahedral point group, such a class of solids was later termed as icosahedral quasicrystals (IQC). If one observes the location of diffracted spots in this class of solids then it is not periodic but all of them are as sharp as any crystalline diffraction patterns. These observations clearly established the fact that IQC displays new type of long range translational order known as Quasiperiodic translational order. We refer the readers to the annotations and reprints of papers in reference [2] for getting familiar with all the terminologies in this area. Having recorded diffraction patterns, the first step is to index them. For indexing, we need a set of basis vectors that are integrally independent. All three dimensionally periodic solids need three integrally independent basis vectors to index their diffraction patterns. The minimum number of integrally independent basis vectors is known as rank of any solids possessing long range translational orders [3-4]. Thus, all 3d periodic solids have rank equals to three. Remember, one uses four basis vectors for hexagonal crystals in Miller-Bravais (MB) scheme but all of them are not independent. As a consequence of this, assignment of indices to a diffracted spot in MB scheme is made unique by invoking condition that sum of indices along the three planar basis vectors is zero. We shall deliberate on this aspect further while discussing indexing of decagonal quasicrystals (DQC).

All Quasiperiodic structures possess rank greater than three. This is true even for incommensurate structures. However, quasicrystals diffraction patterns are invariant under

non-crystallographic point groups that are incompatible with periodic lattice translations. We do not propose to discuss this aspect further and interested readers may refer to international tables on crystallography [5] for subtle distinction between these phases. IQC are three dimensional (3d) quasicrystals whose diffraction patterns are invariant under icosahedral point group. For the purpose of indexing, one requires six integrally independent basis vectors parallel to the vertex vectors of an icosahedron. Thus, 3d IQCs have rank equals to three. We shall demonstrate that all the diffraction spots can be indexed with the help of sextuplets of indices. For spanning the entire reciprocal space one has to follow the rules of addition and subtraction. This is true for all reciprocal lattices. In addition to this, Quasiperiodic reciprocal lattices require inflation and deflation of vectors. We shall show this as we progress. The Quasiperiodic lattice constant is determined with the help of first strongest diffraction spots along the basis vectors. Owing to quasiperiodicity, Quasiperiodic lattice constant is scale dependent. The concepts of inflation/deflation and scale dependent lattice constant are reflection of the fact that we are dealing with a new state of order. In fact both these concepts are related to golden mean $\tau = \frac{\sqrt{5}+1}{2}$ which is one of the roots of the equation $x^2 - x - 1 = 0$. Please note that the golden mean has many interesting properties like $\tau^2 = \tau + 1$, $\left(\frac{1}{\tau}\right) = \tau - 1$, $\tau^3 = 2\tau + 1$ and so on. IQC phases are related to such a number. This is due to the presence of 5-fold rotational symmetry. There are three 6d Bravais lattices for IQC and they are expected to give rise to three distinct icosahedral phases. These are (i) Simple IQC (SI), (ii) Body centered IQC (BCI) and (iii) Face centered IQC (FCI). Both SI and FCI phases are reported in literature but we shall restrict our discussion on SI only. The need of 6d cubic lattice in the structural description of IQC has been found to be essential and convenient in higher dimensional crystallography. It is therefore essential that we get familiarize with the concept and methodology related to higher dimensional crystallography. We shall demonstrate all the necessary aspects pertaining to this as we proceed.

Following the discovery of IQC, a new class of quasicrystals was found. This class of quasicrystals has 2d quasiperiodicity and 1d periodicity. Four popularly known DQCs have 2,4,6 and 8 layer periodicities along 10-fold axis and are designated as T_2 , T_4 , T_6 and T_8 phases respectively. The diffraction pattern displayed the presence of a unique 10-fold symmetry axis. Hence, this class of 2d QC was christened as decagonal quasicrystals. The discovery of decagonal phases [6-7] posed novel problems to their structural description and indexing. The rank of such a solid is five. Four basis vectors oriented with respect to each other by 72° and the fifth one perpendicular to this plane are sufficient to map the entire reciprocal space. However, a set of vectors related by five -fold symmetry may not possess quintuplet of indices that are permuted. These aspects are dealt extensively in references [8-9]. To attain permuted indices to refer to a set of vectors related by 5-/10-fold symmetries one uses six basis vectors [10]. The additional vector required to preserve symmetry in the indices for a family of directions/planes during indexing gives rise to the problem of redundancy. This refers to the non-unique assignment of indices to a diffraction spot. This can be surmounted by putting condition on indices akin to those of MB scheme for hexagonal crystal. We have recently discussed many novel aspects pertaining to this [9] by revisiting the MB indexing schemes of hexagonal [10-11], decagonal [8] and their related phases with the help of higher dimensional approach. For indexing diffraction patterns, one has to follow the approach of Copernican crystallography developed in Fourier space [3, 4].

In contrast, the canonical cut and project scheme [12-17] is capable of providing information about the atomic positions as well as the intensity of Quasiperiodic structures. We will not be deliberating on these in this chapter excepting succinctly dealing with the concepts of higher dimensional crystallography in the next section. Higher dimensional crystallography utilizes a mathematical construct for structural modeling of Quasiperiodic phases in a convenient way.

2. Elements of quasicrystallography

We need to remember that diffraction patterns offer the best way to define a lattice. We may understand this in the following way. If we ignore the intensity variation and replace all the diffracted spots by a point (for example, selected area electron diffraction pattern from a single grain) then we get arrangement of points in 2d section of a 3d reciprocal lattice. The prefix reciprocal before lattice appears because the distances are measured in terms of \AA^{-1} . For describing atomic arrangements of solids one has to express distances in terms of \AA and the underlying lattice is known as direct lattice. A lattice has a set of basis vectors whose integral linear combination helps us reach any diffracted spot with respect to the transmitted beam. Similar concept will hold for direct primitive lattice. The minimum number of integrally independent basis vectors required to accomplish this task is known as the rank of solids. Please note that the way we have introduced lattice does not demand anything other than the existence of diffraction patterns. Latter is a hard verifiable experimental fact. Selected area diffraction is the most convenient way to record single crystal like diffraction patterns from a polycrystalline specimen. Developing crystallography with the help of reciprocal space was central philosophy advocated earlier [18]. This concept was emphasized and extended further by N.D.Mermin (1992) after the discoveries of IQC, DQC and many other related phases [3-4]. If we observe three dimensional periodicities in diffraction patterns then we are dealing with the crystals of rank 3. The observation of incommensurate structures in 1977 [12] and their interpretation demanded four basis vectors instead of three. Incommensurate structures display crystallographic point group symmetry but their diffraction patterns possess aperiodicity in one of the three directions. In contrast, quasicrystals discovered by Shetchman et al. in 1984 displayed icosahedral point group symmetry [1] and aperiodicity of a special type. We call this as quasiperiodicity. In general, the existence of aperiodic order in a direction, demands at least two length scales that are relatively incommensurate. This is said in other words means the ratio of two fundamental lengths cannot be expressed as a rational number. We may understand this in a mathematical way as given below.

Let us consider a point on the line whose distance from an arbitrary origin is X_n . We define this by

$$X_n = a \left(n + (1/\tau) \lfloor (n/\tau) \rfloor \right) \quad (1)$$

Where the floor function $\lfloor x \rfloor$ of any number x is defined by the number x minus the fractional part of x . This means that floor function is basically the lowest possible integer of that number. As a consequence of this we realize that the two terms in the above equation are periodic independently with a period of a and (a/τ) respectively. H.Bohr has shown that equation (1) generates points that are almost periodic or Quasiperiodic [19-20]. The

floor function also ensures that the two consecutive points are not coming arbitrary close to each other. This is important for a real solid. There has to be a minimum distance of separation between two atoms.

Thus, we may write a general expression having aperiodicity as

$$X_{m,n} = a[m + n\tau] \quad (2)$$

Where, m and n are integers.

A simple calculation of X_n based on equation (1) generates points on a line that is well known Fibonacci series for $\tau = 1.618\dots\dots$ (golden mean). This is a quadratic irrational. As mentioned earlier, this is one of the two roots of equation $x^2 - x - 1 = 0$. Golden mean τ has a continued fraction representation: $\tau = 1 + 1/1 + \dots = 1/1; 2/1; 3/2; 5/3; 8/5; 13/8; 21/13$ and so on. These are the successive approximants of τ . One way to generate periodic structures of varying periods is by replacing τ by one of the above rational values. Such structures are known as rational approximants. We proceed to give alternative discussion of equations (1) and (2) in terms of higher dimensional crystallography.

Let us consider a set of points on one dimension of the type that we have been discussing so far. If we have to index each of the points on the lattice generated by equation (1) then we will do it conveniently by specifying two integers (m, n). Thus the rank of such a lattice is 2. Please note that the points are lying on a line. If this happens for a three dimensional solids in all the three directions then we will require 6 indices to indicate a point for such cases. Thus, the rank of such a solid will be 6. This is the case for IQC phase. Let us translate this discussion in terms of basis vectors. We shall first do it for the one dimensional Quasiperiodic case.

Let us consider two vectors V_1 and V_2 along a direction with unit vector x^{par} such that $V_1 = \cos\theta x^{\text{par}}$ and $V_2 = \sin\theta x^{\text{par}}$. Any vector on the line terminating at a lattice point is given by:

$$R = a(m_1 V_1 + m_2 V_2) \quad \text{and} \quad G = (1/a)(n_1 V_1 + n_2 V_2) \quad (3)$$

Where R and G are direct and reciprocal space lattice vectors; m_1, m_2 and n_1, n_2 are set of integers and a is spacing in \AA . For direct space there has to be a minimum separation between two points as every lattice point is a probable location of atom. For reciprocal space this is not at all essential. If we choose $(\cos\theta / \sin\theta) = \tau$, then we have

$$R = a \sin\theta(m_1\tau + m_2) \quad \text{and} \quad G = (1/a) \sin\theta(n_1\tau + n_2) \quad (4)$$

The form of set of equations now resembles with those of equations (1) and (2). If we choose integers that are a combination of positive and negative both then there is an important difference between periodic solids and aperiodic ones. The set of points generated on the line is uniformly and densely filled. For R , this is obviously inconsistent. We commented earlier about the minimum distance of separation between two points. We also know from the experimental observations of IQC that in reciprocal space, we do observe sharp Bragg

peaks at discrete locations just like periodic crystals. Let us attempt to understand this through the language of higher dimensional crystallography. We construct a projection matrix (P) through the dot products of the basis vectors.

$$P = \{P_{ij}\} = \{V_i \cdot V_j\} \text{ where } P_{11} = \cos^2\theta; P_{22} = \sin^2\theta; P_{12} = \cos\theta\sin\theta$$

$$P = \begin{bmatrix} \cos^2\theta & \cos\theta\sin\theta \\ \cos\theta\sin\theta & \sin^2\theta \end{bmatrix} \quad (5)$$

Equation (5) satisfies $P^2 = P$. This is an important property of a projection matrix. Please note that the determinant of this matrix is zero and the trace is equal to 1. We can also define a matrix Q by the following relation:

$$Q = I - P = \begin{bmatrix} \sin^2\theta & -\sin\theta\cos\theta \\ -\sin\theta\cos\theta & \cos^2\theta \end{bmatrix} \quad (6)$$

Where I is an identity matrix of order 2. Please see that $Q^2 = Q$ and $PQ = 0$. All other properties of P are displayed by Q also. The space generated by this matrix is orthogonal to that of P .

If we choose another set of basis vectors W_1 and W_2 then we are in a position to define these on a line such that they are anti-parallel or at 180° with each other. Please note that in parallel space V_1 and V_2 are parallel. From the learning of matrix representation theory, we call the two spaces to be orthogonal. In terms of a unit vector x^{perp} we may write $W_1 = \sin\theta x^{\text{perp}}$ and $W_2 = -\cos\theta x^{\text{perp}}$.

We may define a orthonormal basis such that $V_i + W_i = e_i$ where $i = 1$ to 2 and $e_i e_j = \delta_{ij}$ with $\delta_{ij} = 1$ for $i=j$ and $\delta_{ij} = 0$ for $i \neq j$. The two basis vectors e_1 and e_2 are orthonormal and clearly represent the bases for a two dimensional space. With the help of two matrices given in equations (5 and 6), we can also write $V_i = P_{ij} e_j$ and $W_i = Q_{ij} e_j$ for i, j to vary from 1 to 2 only. The two dimensional direct lattice vector R^2 and reciprocal lattice vectors G^2 can now be written as:

$$R^2 = a (m_1 e_1 + m_2 e_2) \text{ and } G^2 = (1/a)(n_1 e_1 + n_2 e_2) \quad (7)$$

Where a can be identified as two dimensional lattice parameter of a square lattice. Let us designate now R and G as the components of Equation (7) in "V" space or "physical space" or "par space" and S and H as the components of Equation (7) in "W" space or "pseudo space" or "complementary space" or "perp space". All these terminologies are used in Quasicrystalline literature and we need not get frightened by them. They are given by

$$R = a (m_1 V_1 + m_2 V_2) \text{ and } G = (1/a)(n_1 V_1 + n_2 V_2) \quad (8)$$

$$S = a (m_1 W_1 + m_2 W_2) \text{ and } H = (1/a)(n_1 W_1 + n_2 W_2) \quad (9)$$

We get after substituting for V_i and W_i the following expressions:

$$R = a \sin\theta (m_1 \tau + m_2) x^{\text{par}} \quad (10a)$$

$$G = (1/a)\sin\theta (n_1\tau + n_2) X^{par} \quad (10b)$$

$$S = a\sin\theta (m_1 - m_2\tau) X^{perp} \quad (11a)$$

$$H = (1/a)\sin\theta (n_1 - n_2\tau) X^{perp} \quad (11b)$$

We observe that the terms within the parentheses of equations (10a) and (10b) are of the same form as we have written earlier in equations (1) and (2). Are we getting any extra information by following the path that we have adopted in the latter part of the discussion? Yes, we can ensure minimum separation between two points in the direct lattice if we put a condition on the set of indices m_1 and m_2 with the help of equation (11a). Please recall that the floor function in equation (1) was helping us accomplish this task. The matrix formulation presented here can be generalized without any difficulty for two and three dimensional aperiodic structures or Quasiperiodic structures for our discussion.

As mentioned above, we demonstrate the method of ensuring minimum distance of separation between two points in parallel or physical direct space. We have a square 2d lattice (we call them as hyperlattice) having basis vectors e_1 and e_2 with lattice parameter a . We attach a line element to each of the lattice points. The length of the line element is L^{perp} (say). Please note that (L^{perp}/a^2) is the linear density of points. We choose this based on the density of the points required for the purpose. This can be arrived at by referring to the density of the points needed for the related approximant structures. As stated earlier, structures that are generated by substituting τ by its successive approximants are termed as rational approximant structures. The α -Al-Mn(Fe)-Si cubic structure with space group Pm3 having lattice parameter of $\sim 12.68\text{\AA}$ and 138 atoms in the unit cell is one such example. This is described as (1/1) approximant of icosahedral structures in Al-Mn system. Please see annotations in reference [2] and also consult [21] for further details.

In cut and project scheme, the length of such a line element is taken as $L^{perp} = a(\sin\theta + \cos\theta)$. This is the external boundary of the shape in W -space obtained by projecting all the vertices of the higher dimensional unit cell on to it. We place it on the lattice point such that it is parallel to $perp.space$ and is symmetric around it. This means the line element is extending both sides from $+(L^{perp}/2)$ to $-(L^{perp}/2)$. We may also work with the asymmetric setting by placing the line element having its extent from 0 to L^{perp} . The physical space line will cut this line element selectively and minimum separation between the two consecutive points can be ensured [14-16]. Now we would like to understand the *Fourier Transform (F.T.)* of the structure that we have generated. It is a combined effect of two distinct entities: the 2d square hyperlattice and the line element L^{perp} that is serving as motif in crystallographic parlance. Hence the *F.T.* of the 1d quasicrystals in physical space will be given by the convolution of the two functions. The *F.T.* of the 2d lattice will be a delta function and the weight of the delta function will be modulated by the *F.T.* of the line element. We therefore write:

F.T. of the 1d Quasicrystals = F.T. of the 2d lattice \times F.T. of the line element

$$F.T.(G) = 1 \times (1/L^{perp}) \int_{-(L^{perp}/2)}^{(L^{perp}/2)} \text{Exp}(-2\pi i H.S) dS \quad (12)$$

This reduces to

$$F.T.(G) = (\sin \pi H L^{perp}) / (\pi H L^{perp}) \quad (13)$$

For a given G , there is a unique H and are given by indices of reflection

$(n_1 n_2)$. The intensity is given by the following equation:

$$I(G) = F.T.(G) \times F.T.(G)^* \quad (14)$$

Where $F.T.(G)^*$ is the complex conjugate of $F.T.(G)$. Please note that G and H are implicitly and uniquely related. The right hand side of the equation (13) will try to attain maximum value for those G for which H is close to zero. In experimental condition, the instrument has a cut off limit below which it will merge with the background. Hence most of the intensities may not be significant. The observed G with reasonable intensity shall correspond to only those G 's for which n_1/n_2 is nearing to τ . This is the reason why we observe sharp Bragg peaks at discrete locations in physical or parallel reciprocal space under experimental condition. Having explained the philosophy for 1d case, we come back to the indexing of diffraction patterns again—the primary aim of this paper. We reproduce the two expressions again:

$$G = (1/a) \sin \theta (n_1 \tau + n_2) x^{par} \text{ and } H = (1/a) \sin \theta (n_1 - n_2 \tau) x^{perp}$$

Please note that $(n_1 - n_2 \tau) \rightarrow 0$ when $(n_1/n_2) \rightarrow \tau$. Thus all the diffracted vectors having significant observable intensities will be indexed as $(1,1);(2,1);(3,2);(5,3)$ and so on. If we follow similar arguments for 3d or 2d Quasiperiodic solids, we may conclude that icosahedrally related structures will display strong intensity spots separated by τ or its power dependent on the symmetric direction(s). All those solids having τ or its successive approximants playing a role in the diffraction patterns are important for icosahedrally related structures. We advise readers to consult books and reviews available in this area through various scientific databases for further details on this aspect.

3. Icosahedral quasicrystals

As mentioned above, we have 3d quasiperiodicity for IQC and we need 6 integrally independent basis vectors to index the diffraction patterns. The rank of this class of solids is six. Recall that icosahedron is one of the five platonic solids having 20 equilateral triangles giving it a convex shape. It has 6 (or 12) five-, 10 (or 20) three- and 15 (or 30) two- fold axes. They are respectively the vertex, face and edge vectors of an icosahedron. The angular relationships amongst them can be known by referring to stereographic projection of icosahedral point group symmetry given in Figure 1. The icosahedral point group is $(m\bar{3}5)$ and the order of the group is 120. If we ignore inversion then it is of order 60. Please note that number of vertex vectors and rank are the same. Hence six vertex vectors of an icosahedron can serve as the six integrally independent basis vectors. All the diffracted spots are indeed seen to be expressible in terms of six integers. We shall designate such a sextuplet of indices as $(n_1 n_2 n_3 n_4 n_5 n_6)$ and six basis vectors (vertex vectors) by V_1, V_2, V_3, V_4, V_5 and V_6 . We may express these in relation to three Cartesian bases (x^{par}, y^{par} and z^{par}) in physical or parallel space by the following matrix relation.

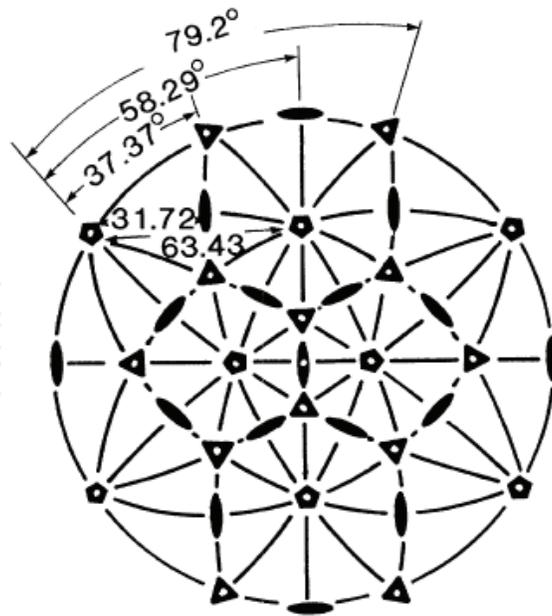


Fig. 1. Stereographic projection of the symmetry elements of the icosahedral point group

$$\begin{pmatrix} V_1 \\ V_2 \\ V_3 \\ V_4 \\ V_5 \\ V_6 \end{pmatrix} = \frac{1}{\sqrt{2(1+\tau^2)}} \begin{bmatrix} \tau & 1 & 0 \\ 0 & \tau & 1 \\ -1 & 0 & \tau \\ 0 & -\tau & 1 \\ \tau & -1 & 0 \\ 1 & 0 & \tau \end{bmatrix} \begin{pmatrix} x^{par} \\ y^{par} \\ z^{par} \end{pmatrix} \quad (15)$$

It is obvious that the magnitudes of all the vertex vectors are equal. $|V_1| = |V_2| = |V_3| = |V_4| = |V_5| = |V_6| = (1/\sqrt{2})$. V_6 is the polar vector in this setting and $\sum_1^5 V_i = (2\tau - 1)V_6$. Thus a vector represented by the sextuplets (111112) is a five-fold vector parallel to V_6 with a magnitude of τ^3 times that of V_6 . There are five distinct set of equivalent choices for choosing a set of three Cartesian bases as there are fifteen two fold vectors in icosahedron. The orientation and magnitude of vectors are known directly by the projection matrix P^{icos} . One may write the elements of this matrix by dot or scalar product of basis vectors (Cf. section 2) and is given by

$$P^{icos} = \left(\frac{1}{\sqrt{20}} \right) \begin{pmatrix} \sqrt{5} & 1 & -1 & -1 & 1 & 1 \\ 1 & \sqrt{5} & 1 & -1 & -1 & 1 \\ -1 & 1 & \sqrt{5} & 1 & -1 & 1 \\ -1 & -1 & 1 & \sqrt{5} & 1 & 1 \\ 1 & -1 & -1 & 1 & \sqrt{5} & 1 \\ 1 & 1 & 1 & 1 & 1 & \sqrt{5} \end{pmatrix} \quad (16)$$

Please note all the diagonal elements are equal and $V_i \cdot V_i = (1/4)$ and the trace of the matrix is 3. The projection matrix P^{icos} has the property as mentioned in section 2. The angle between V_i ($i=1$ to 5) with V_6 is $\cos^{-1}(1/\sqrt{5})$. The matrix elements in Equation (16) has all the information about the metrical and symmetrical properties of basis vectors. We shall extensively utilize this equation for knowing a direction of SADP of IQC. We can also write the projection matrix Q^{icos} in the complementary or pseudo or perpendicular space as:

$$Q^{icos} = I - P^{icos} = \left(\frac{1}{\sqrt{20}} \right) \begin{pmatrix} \sqrt{5} & -1 & 1 & 1 & -1 & -1 \\ -1 & \sqrt{5} & -1 & 1 & 1 & -1 \\ 1 & -1 & \sqrt{5} & -1 & 1 & -1 \\ 1 & 1 & -1 & \sqrt{5} & -1 & -1 \\ -1 & 1 & 1 & -1 & \sqrt{5} & -1 \\ -1 & -1 & -1 & -1 & -1 & \sqrt{5} \end{pmatrix} \quad (17)$$

Please note that trace of Q^{icos} is 3 and we can see that polar vector W_6 (complementary vector of V_6 in perp.space) is inverted with respect to other vectors in perp. space. We designate the perp.space basis vectors by W_1, W_2, W_3, W_4, W_5 and W_6 . We may express these in relation to three Cartesian bases (x^{perp}, y^{perp} and z^{perp}) in physical space by the following matrix relation.

$$\begin{pmatrix} W_1 \\ W_2 \\ W_3 \\ W_4 \\ W_5 \\ W_6 \end{pmatrix} = \frac{1}{\sqrt{2(1+\tau^2)}} \begin{bmatrix} 1 & -\tau & 0 \\ 0 & 1 & -\tau \\ \tau & 0 & 1 \\ 0 & -1 & -\tau \\ 1 & \tau & 0 \\ -\tau & 0 & 1 \end{bmatrix} \begin{pmatrix} x^{perp} \\ y^{perp} \\ z^{perp} \end{pmatrix} \quad (18)$$

The magnitude of all the vectors (W_1, W_2, W_3, W_4, W_5 and W_6) is same and is equal to $(1/\sqrt{2})$. This is just like that of *par* space basis vectors mentioned earlier. V- and W- spaces possess vector like and non-vector like representations respectively. Any 5- fold rotation around V_6 takes $V_1 \rightarrow V_2 \rightarrow V_3 \rightarrow V_4 \rightarrow V_5 \rightarrow V_1$ whereas that around W_6 takes $W_1 \rightarrow W_3 \rightarrow W_5 \rightarrow W_3 \rightarrow W_4 \rightarrow W_1$. Such spaces are said to be orthogonal in matrix representation [see annotations in reference 2]. Please note the way, we have defined the projection matrices here, permits us to write the decomposition of the 6d hyperspace orthonormal basis vectors e_i ($i=1$ to 6) in terms of two complementary 3d spaces basis vectors as explained in section 2. This is given by

$$e_i = V_i + W_i \quad (19)$$

$$V_i = P^{icos}_{ij} e_j \text{ and } W_i = Q^{icos}_{ij} e_j \quad (20)$$

$$P^{icos}_{ij} + Q^{icos}_{ij} = I_{ij} \quad (21)$$

Where, I_{ij} is an identity matrix of order 6.

The 6d direct hypercubic lattice vector is given by

$$R^6 = t^{\text{icos}} \sum_1^6 m_i e_i \quad (22)$$

The 6d reciprocal lattice vector is written as

$$G^6 = (1/t^{\text{icos}}) \sum_1^6 n_i e_i \quad (23)$$

Where m_i and n_i are integers and t^{icos} is the 6d hypercubic lattice parameter. The physical or parallel and pseudo or perpendicular space components are written in a straight forward manner owing to the identity given by equation (19). They are

R^{icos} = parallel space component of R^6

$$= t^{\text{icos}} \sum_1^6 m_i V_i \quad (24)$$

S^{icos} = perpendicular space component of R^6

$$= t^{\text{icos}} \sum_1^6 m_i W_i \quad (25)$$

G^{icos} = parallel space component of G^6

$$= (1/t^{\text{icos}}) \sum_1^6 n_i V_i \quad (26)$$

H^{icos} = perpendicular space component of G^6

$$= (1/t^{\text{icos}}) \sum_1^6 n_i W_i \quad (27)$$

For indexing, the relevant expression is given by equation (26) and any diffracted spot or peak is represented by the sextuplet of indices $(n_1 n_2 n_3 n_4 n_5 n_6)$. Equation (26) can also be written with the help of matrix given in equation (15) in the following way:

G^{icos} = parallel space component of G^6

$$= (1/t^{\text{icos}}) (1/\sqrt{2(1+\tau^2)}) (G_x x^{\text{par}} + G_y y^{\text{par}} + G_z z^{\text{par}}) \quad (28)$$

Where,

$$G_x = \tau (n_1 + n_5) + (n_6 - n_3)$$

$$G_y = \tau (n_2 - n_4) + (n_1 - n_5) \quad (29)$$

$$G_z = \tau (n_3 + n_6) + (n_2 + n_4)$$

Please note that a vector (000001) is parallel to V_6 . Also, a vector (111112) is τ^3 times that of V_6 . These are known as τ^3 inflation rule along the five-fold axis. The inflation matrix can be written for this purpose as

$$\begin{pmatrix} 2 & 1 & -1 & -1 & 1 & 1 \\ 1 & 2 & 1 & -1 & -1 & 1 \\ -1 & 1 & 2 & 1 & -1 & 1 \\ -1 & -1 & 1 & 2 & 1 & 1 \\ 1 & -1 & -1 & 1 & 2 & 1 \\ 1 & 1 & 1 & 1 & 1 & 2 \end{pmatrix}$$

We may write the deflation matrix by inverting it. We also note that for the two fold and three fold directions, the following inflation relations hold:

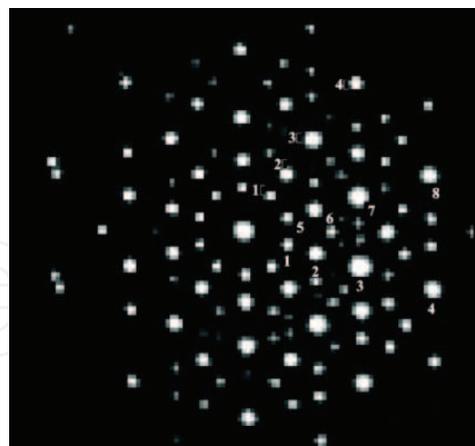
$$\text{2-fold vector: } (001001) = \tau (010100)$$

$$\text{3-fold vector: } (011001) = \tau^3 (1001\bar{1}0)$$

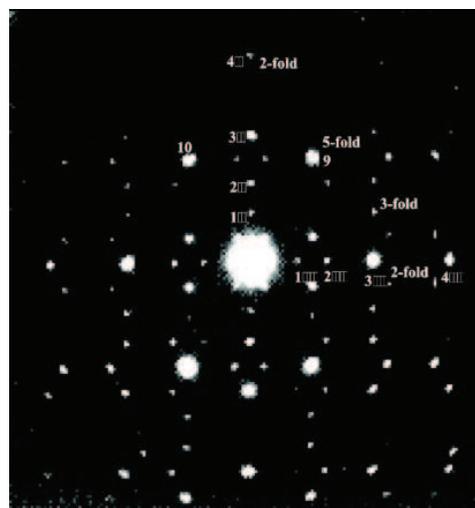
We may write the indices of any reflections by inflation and deflation along any direction with respect to first strongest spot that one encounters with respect to transmitted beam in SADP. The principal zone axes (5,-3- and 2-fold directions) can be easily recognized by looking at rotational invariance of diffraction pattern. Please see Cahn et al. (1986) for this purpose [22].

We enlist steps that may be followed for indexing any SADP pattern of IQC. We show three SADPs of IQC in Figure 2. Figure 2a is invariant under five-fold rotation. We call this pattern belonging to a five-fold zone. We consider a 72° sector of this SADP. We observe two spots of same intensities at same reciprocal distance from the transmitted beam along the two 2-fold directions oriented at 72° . All the vertex vectors are 5-fold vectors. We therefore may designate this zone by any one of these. Let us designate this zone as [000001]. We would like to know a set of vectors that are orthogonal to this. All the 2-fold vectors $[1\bar{1}0000]$, $[10\bar{1}000]$, $[100\bar{1}00]$, $[1000\bar{1}0]$, $[01\bar{1}000]$, $[010\bar{1}00]$, $[0100\bar{1}0]$, $[001\bar{1}00]$, $[0010\bar{1}0]$, and $[0001\bar{1}0]$ are orthogonal to [000001]. One may verify this by looking at the dot products from equation (16). Hence, all these 20 (10 negatives of these two fold vectors) are lying in the zone. Out of these five 2-fold vectors $[100\bar{1}00]$, $[0100\bar{1}0]$, $[0\bar{1}0100]$, $[00\bar{1}010]$, and $[\bar{1}01000]$ are oriented with respect to each other at 72° in this zone. Owing to scaling property, assignment of indices to the first strongest spot may be done by recalling the nature of appearance of spots. Along the two fold axes, the location of spots follows τ -scaling. The inflation matrix corresponding to τ -scaling is given by

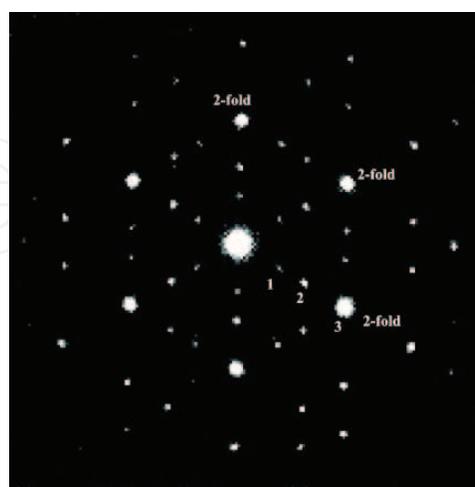
$$(1/2) \begin{pmatrix} 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & -1 & 1 \\ -1 & 1 & 1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}$$



(a)



(b)



(c)

Fig. 2. Selected area diffraction pattern from simple icosahedral phase under (a) 5-fold (b) 2-fold and (c) 3-fold zones. Indices of the important spots are given in Table 1.

The first spot along one of the aforesaid five 2-fold directions can be indexed as $[001\bar{1}00]$ and if we take help of above matrix then next spot after inflation by τ will be $[0100\bar{1}0]$. Likewise we may index spots that are lying along a two-fold direction $[0\bar{1}0100]$ at 72° to $[0100\bar{1}0]$. Having done this we may utilize the rules of vector addition to index spots that are lying within 72° sector. We tabulate the indices of spots based on these steps in table 1a.

Let us try to index spots in a 2-fold zone now (see Fig. 2b). Consider a 2-fold zone $[001001]$. Please note that this is parallel to Z-axis and all the diffraction vectors having only X-Y components will be contained in this zone. The sextuplets of indices corresponding to 2-fold $[00\bar{1}001]$ and $[100010]$ are parallel to X-axis and are related by τ -scaling. Similarly, the 2-fold vectors $[1000\bar{1}0]$ and $[010\bar{1}00]$ are parallel to Y-axis. Latter is τ time more than the former. We see strong spots at $(1/2) \cos^{-1}(1/\sqrt{5}) \sim 31.7^\circ$ orientation with respect to these 2-fold directions that are lying along 5-fold directions. From the geometrical relationships of 3-fold and 5-fold vectors, we identify a direction in the 2-fold zone at 37.37° . The 3-fold directions $[110\bar{1}00]$ and $[00\bar{1}0\bar{1}1]$ are parallel to each other and are related by τ^3 -scaling. The dot product of these 3-fold vectors with $[001001]$ is zero. Hence such a 3-fold direction is contained in this zone. The indices of diffracted spots in 2-fold zone are given in table 1b. Having done this exercise, the indexing of spots in 3-fold zone is straight forward as it contains 2-fold vectors and their addition/subtraction (see Fig. 2c). Please note that spots indicated along one of the two fold directions in this figure have the similar spot designations akin to those of Figure 2a. As a consequence of this, their indexing remains the same. It is important to mention here that the 2-fold zone axis from IQC is important as it contains 2-fold, 3-fold and 5-fold directions. If one is able to get this zone at zero tilt position while recording SADP then with the help of tilt, one will be able to visit all the principal zone axes by recalling orientation of various symmetry directions with the help of Fig. 1.

(a) 5-fold zone axis $[000001]$					
Spot No.	Indices	Spot No.	Indices	Spot No.	Indices
1	$001\bar{1}00$	1'	$0001\bar{1}0$	5	$\bar{1}10000$
2	$0100\bar{1}0$	2'	$\bar{1}01000$	6	$0010\bar{1}0$
3	$011\bar{1}\bar{1}0$	3'	$\bar{1}011\bar{1}0$	7	$\bar{1}110\bar{1}0$
4	$021\bar{1}\bar{2}0$	4'	$\bar{2}021\bar{1}0$	8	$\bar{1}120\bar{2}0$
(b) 2-fold zone axis $[001001]$					
1''	100010	1'''	$010\bar{1}00$	9	$21\bar{1}\bar{1}11$
2''	$10\bar{1}011$	2'''	$110\bar{1}\bar{1}0$	10	$1\bar{1}\bar{1}121$
3''	$20\bar{1}021$	3'''	$120\bar{2}\bar{1}0$	3-fold (τ^3 inflated)	$44\bar{1}4\bar{1}1$
4''	$30\bar{2}032$	4'''	$230\bar{3}\bar{2}0$		

Table 1. Sextuplets of indices assigned to various spots for Icosahedral phase

How to identify the first vector in five-fold direction? As explained earlier, we do not have a fixed magnitude of the vector to identify owing to the nature of expressions given in equation (29). However, this can be settled by identifying the appropriate approximant for a particular type of quasicrystals [13]. For example, the approximant corresponding to Al-Mn type IQC, is the cubic α -Al-Mn-Si structure with space group $Pm\bar{3}$ and lattice parameter $\sim 12.68\text{\AA}$. Reflections having $h+k+l=\text{odd}$, are weak. This is due to the large motif (having icosahedral symmetry) in the unit cell. We observe a strong spot corresponding to a plane at

a distance of $\sim 2\text{\AA}$ having indices $\{530\}$. These are oriented at an angle of $\sim 31^\circ$ ($=\text{Cos}^{-1}(5/\sqrt{34})$) with respect to cubic axes. As mentioned earlier, the angle between the 2-fold and 5-fold is $= (1/2) \cos^{-1}(1/\sqrt{5}) \sim 31.7^\circ$. Thus, the first strongest reflection corresponding to interplanar spacing of $\sim 2\text{\AA}$ along the 5-fold axis in IQC for this alloy system can be indexed as (000001) or its τ^3 inflated value (111112). This problem is unlike that of a crystal [cf. 22]. We have deliberated on this while introducing the subject with the help of 1d example. As mentioned earlier, the intensity of any reflection will be governed by the Fourier Transform of the motif lying in perpendicular space. The symmetry of the motif must conform to the point group of the diffraction patterns. Thus, analysis of diffraction patterns is the first step towards structural modeling.

4. Decagonal quasicrystals

It has been emphasized earlier by us [17, 23-24] that a distorted icosahedral basis vectors are the best to establish relation between the icosahedral and two dimensional Quasiperiodic structures having 10-fold and 5-fold symmetries. A distortion along one of the six five-fold axes of an icosahedron preserves a five-fold symmetry along it. For continuity, the basis vectors utilized by us earlier are reproduced below:

$$V_i = |V_i| [\sin \theta_D T^{i-1} X^{||} + \cos \theta_D Z^{||}] \quad (30)$$

$$V_6 = |V_6| Z^{||}$$

where V_i ($i = 1$ to 5) are parallel to the vertex vector of an icosahedron and V_6 is the sixth vertex vector along which distortion can be given by taking value of $\cos \theta_D$ different from $\frac{1}{\sqrt{5}}$. For this choice, an ideal icosahedral basis vectors are recovered in physical space [14-15]. A symmetric projection matrix can be constructed through the dot product of vectors given in equation (30). The matrix P has the following form

$$P = \begin{bmatrix} P_{11} & P_{12} & P_{13} & P_{13} & P_{12} & P_{16} \\ P_{12} & P_{11} & P_{12} & P_{13} & P_{13} & P_{16} \\ P_{13} & P_{12} & P_{11} & P_{12} & P_{13} & P_{16} \\ P_{13} & P_{13} & P_{12} & P_{11} & P_{12} & P_{16} \\ P_{12} & P_{13} & P_{13} & P_{12} & P_{11} & P_{16} \\ P_{16} & P_{16} & P_{16} & P_{16} & P_{16} & P_{66} \end{bmatrix} \quad (31)$$

where

$$P_{11} = V_1 \cdot V_1 = \frac{2}{5 \sin^2 \theta_D};$$

$$P_{12} = P_{11} \left[\frac{1}{2\tau} \sin^2 \theta_D + \cos^2 \theta_D \right]; \quad P_{13} = P_{11} \left[-\frac{\tau}{2} \sin^2 \theta_D + \cos^2 \theta_D \right];$$

$$P_{16} = |V_1| |V_6| \cos \theta_D;$$

$$P_{44} = V_6 \cdot V_6 = \frac{5}{2} |V_1|^2 (1 - 3 \cos^2 \theta_D) \text{ and } \tau = \frac{\sqrt{5} + 1}{2}.$$

This matrix permits 6d orthonormal basis to define the physical or parallel ($||$) space bases as given in equation (30). For details, readers are referred to our earlier work [17]. The projection matrix Q in the complementary or pseudo or perpendicular (\perp) space is given by $Q = I - P$ where I is an identity matrix of order 6. The corresponding basis vectors in \perp space are written as

$$W_i = |W_1| [\sin \phi T^{(2i-1)} X^\perp + \cos \phi Z^\perp] \quad (32)$$

$$W_6 = |W_6| Z^\perp$$

where $|W_1|^2 = 1 - |V_1|^2$; $|W_6|^2 = 1 - |V_6|^2$; $\cos \phi = \left[\frac{1 - 3 \cos^2 \theta_D}{3 - 5 \cos^2 \theta_D} \right]^{1/2}$; and

$i = 1$ to 5 and $\langle 2i - 2 \rangle$ is modulo 5 . The 6d reciprocal lattice vector G^6 in terms of orthonormal basis vectors (e_i for $i = 1$ to 6) for orthogonal cell [17] is written as

$$G^6 = \frac{1}{t_1} \sum_1^5 N_i e_i + \frac{1}{t_6} N_6 e_6 \quad (33)$$

where t_1 and t_6 are hyperlattice parameters for the 6d orthogonal cell.

The 3d parallel ($||$) and perpendicular (\perp) spaces are denoted here by $G^{||}$ and G^\perp respectively. They are given by following equations

$$G^{||} = \frac{1}{t_1} \sum_1^5 N_i V_i + \frac{1}{t_6} N_6 V_6 \quad (34)$$

$$G^\perp = \frac{1}{t_1} \sum_1^5 N_i W_i + \frac{1}{t_6} N_6 W_6$$

where N_i 's are indices of reflections.

Similarly, the 6d direct space lattice vector (R^6) is written as

$$R^6 = t_1 \sum_1^5 M_i e_i + t_6 M_6 e_6 \quad (35)$$

The parallel and perpendicular space components of R^6 are designated here by R^{\parallel} and R^{\perp} respectively. They are depicted in the form of equations below.

$$R^{\parallel} = t_1 \sum_1^5 M_i V_i + t_6 M_6 V_6 \quad (36)$$

$$R^{\perp} = t_1 \sum_1^5 M_i W_i + t_6 M_6 W_6$$

where M_i ($i = 1$ to 6) are integers. The product

$$\begin{aligned} G^{\parallel} \cdot R^{\parallel} &= P_{11} \sum_1^5 M_i N_i + P_{66} M_6 N_6 + P_{12} N_{12} + P_{13} N_{13} \\ &+ \frac{t_1}{t_6} P_{16} N_6 \sum_1^5 M_i + \frac{t_6}{t_1} P_{16} M_6 \sum_1^5 N_i \end{aligned} \quad (37)$$

where

$$\begin{aligned} N_{12} &= N_1(M_2 + M_5) + N_2(M_1 + M_3) + N_3(M_2 + M_4) \\ &+ N_4(M_3 + M_5) + N_5(M_1 + M_4) \\ N_{13} &= N_1(M_3 + M_4) + N_2(M_4 + M_5) + N_3(M_5 + M_1) \\ &+ N_4(M_1 + M_2) + N_5(M_2 + M_3) \end{aligned}$$

For the icosahedral phase $\cos \theta_D = \frac{1}{\sqrt{5}}$ and $t_1 = t_6$, hence $P_{11} = \frac{1}{2}$; $P_{12} = \frac{1}{2\sqrt{5}}$; $P_{13} = -\frac{1}{2\sqrt{5}}$; $P_{16} = \frac{1}{2\sqrt{5}}$ and $P_{66} = \frac{1}{2}$. This reduces equation (37) as

$$2\sqrt{5} G^{\parallel} \cdot R^{\parallel} = \sqrt{5} \sum_1^6 M_i N_i + (N_{12} - N_{13} + N_{16}) \quad (38)$$

where,

$$N_{16} = \left[N_6 \sum_1^6 M_i + M_6 \sum_1^5 N_i \right]$$

The right hand side of equation (38) has rational and irrational parts. Hence, left hand side cannot be equated to zero to recover exact zone rule that is applicable for crystals. However, this can be made to accept values nearer to zero and for special set of $(N_1 N_2 N_3 N_4 N_5 N_6)$ corresponding to chosen symmetric direction (like 2-fold, 3-fold and 5-fold), it may display

exactly zero. We have already seen example of latter in section 3. Thus, quasiperiodic phases will have the notion of exact and nearly exact zone axes. The purpose of this section is to discuss the structural characteristics of 2d-quasiperiodic structures belonging to two distinct classes (Viz. $P10_5/mcm$; $P10/mmm$).

The planar pentagonal scheme [25-28, 8], in the model of Mandal and Lele [17] corresponds to $\theta_D = 90^\circ$. This leads to $P_{11} = 2/5$; $P_{12} = \frac{1}{5\tau}$; $P_{13} = -\tau/5$; $P_{16} = 0$ and $P_{66} = 1$. Substituting these values in equation (37) gives

$$5G^{\parallel} \cdot R^{\parallel} = \left[2 \sum_1^5 M_i N_i + 5 \sum_1^6 M_6 N_6 - N_{12} \right] + \tau (N_{12} - N_{13}) \quad (39)$$

The absence of N_{16} term for this case is due to the fact that $P_{16} = 0$ (cf. equation 31). Hence,

for this case $\sum_1^5 V_i = 0$. This condition gives rise to problem of non-uniqueness in

indexing. The uniqueness can be ensured by imposing $\sum_1^5 N_i = -2$ to $+2$. Equation (39)

is satisfied for diffraction patterns corresponding to $10/m$ symmetry. It is clear that such bases are devoid of group-subgroup relationship with the icosahedral phase in view of severe distortion of the icosahedron. This aspect has been dealt while discussing interfaces and twinning in quasiperiodic structures [29-31].

There are experimental observations of two separate classes of decagonal phases [32-36]. They are having space groups $P10_5/mcm$ and $P10/mmm$. The presence of screw in the former case necessarily demands preservation of $\bar{5}$ symmetry in their bases. Such a choice will generate structures that are maintaining group-subgroup relationship with the icosahedral phase. This will also include $P10_5/mcm$. Please note that for this case, the bases will satisfy the following general condition

$$\sum_1^5 V_i = 5 \cos \theta_D |V_1| Z^{\parallel} \quad (40)$$

A choice of $\cos \theta_D = \frac{1}{2}$ has been shown to conform to the experimentally observed structures having $P10_5/mcm$ space group [23]. The structural details of this class in terms of 5d Patterson map can be found elsewhere [37-38].

Owing to equation (40), the indexing would require imposition of condition on the sextuplet rather than the quintuplet corresponding to $\theta_D = 90^\circ$. It is to be remembered here that different nature of group-subgroup relationships that the two classes of decagonal phases maintain with those of icosahedral structures are expected to reflect upon the condition of uniqueness on indices. Such a condition for $\theta_D = 60^\circ$ can be achieved by recalling that $G^{\parallel}(2222\bar{5}) = 0$ and $R^{\parallel}(1111\bar{4}) = 0$ [23-24]. Hence, the conditions on indices are

$$\sum_1^6 N_i = 0 \text{ modulo } 5$$

$$= -2, -1, 0, 1, 2$$

and

$$\sum_1^6 M_i = 0$$

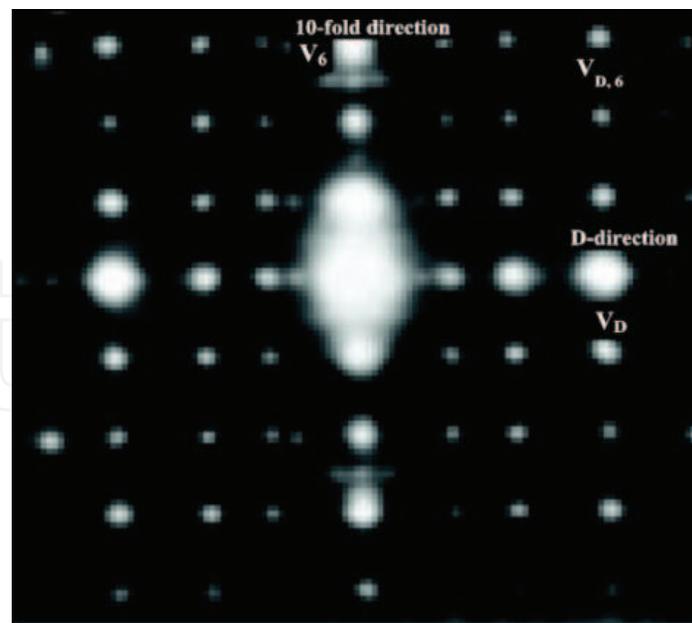
For $\cos \theta_D = \frac{1}{2}$; $P_{11} = \frac{8}{15}$; $P_{12} = \frac{3\tau-1}{15}$; $P_{12} = P_{13}$; $P_{16} = \frac{1}{3} \sqrt{\frac{2}{5}}$; $P_{66} = \frac{1}{3}$;
 $(t_1/t_6) = 2\sqrt{2/5}$.

Hence, Equation (37) for this case reduces to

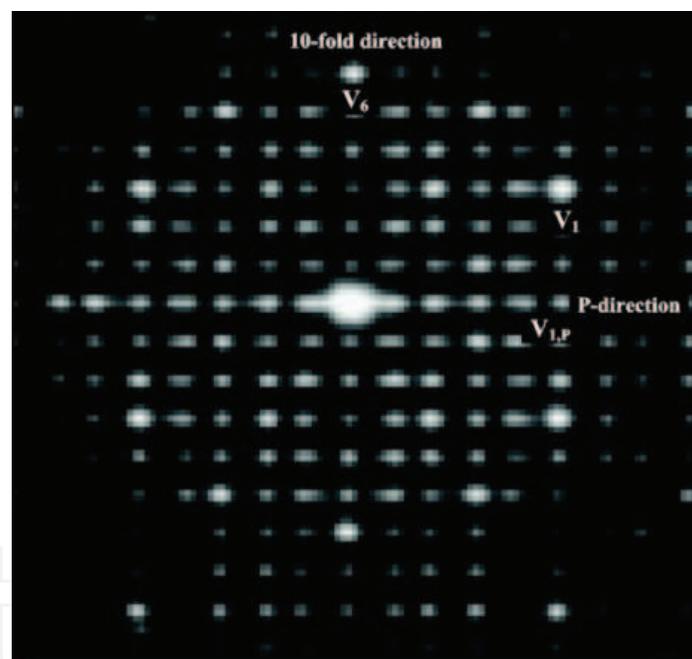
$$30 G^{\parallel} \cdot R^{\parallel} = \left[16 \sum_1^5 M_i N_i + 10M_6 N_6 - 2(N_{12} - N_{13}) \right. \\ \left. + 8N_6 \sum_1^5 M_i + 5M_6 \sum_1^5 N_i \right] + 6\tau [N_{12} - N_{13}] \quad (41)$$

Equation (41) is depiction of zone rule for P10₅/mcm structure corresponding to $\cos \theta_D = 1/2$. The right hand side of equation (41) has quadratic irrational. For those zone axes for which term containing quadratic irrational is absent, one will fulfill exact zone condition. Recording diffraction patterns corresponding to such zones is essential for determination of point group symmetry of the reciprocal space. For this, the quality of thin foil has to be good so that tilt experiment can be conducted during transmission electron microscopic studies of quasicrystals both in imaging and diffraction modes. We are making these specific statements to clarify that quasicrystals are normally brittle materials and for making thin foil one should devote time. Having achieved this, we have to conduct diffraction and imaging experiments to uniquely settle its existence to rule out the possibility of irrational twins. Kindly recall while arriving at zone rule in equation (39) for $\theta_D = 90^\circ$ (P10/mmm structure) the ratio of (t_1/t_6) was not required. This indicates (t_1/t_6) may not be fixed for P10/mmm phase. In contrast, quantification of zone rule for P10₅/mcm types of structure requires a priori prescription of (t_1/t_6) ratio. Thus the two Quasiperiodic structures having periodicity in one dimension of similar type [32-35] demand different types of hyperlattice parameters. This distinction has to be kept in mind while discussing these structures [9].

Having discussed zone rules of various Quasiperiodic structures, we proceed to index SADPs of decagonal phase. The unique 10-fold pattern containing 2-fold axes can be indexed by noting two distinct set of 2-fold directions. These are termed as P- and D-direction respectively. They are oriented with respect to each other at 18⁰ intervals. Let us try to identify them with the help of two characteristics patterns viz. P- and D- patterns. We show them in Figures 3a and 3b. Both these patterns have 10-fold direction. We see strongest



(a)



(b)

Fig. 3. Selected area diffraction patterns from decagonal phase (T_6) under two 2-fold zones (a) P-pattern and (b) D-pattern. The indices of important spots are given in Table 2.

spots (V_6) along this. There are 3 and 6 intervals between transmitted spots and V_6 respectively in P- and D- patterns. In P-pattern, odd rows have streaking while those in D-pattern are weak spots. We expect nearly absence of odd rows in P-pattern due to 10_5 screw. However, this may not be the case for D-pattern owing to presence of diffraction vectors of the type V_1 . The strongest spot along 10-fold axis getting divided into six equal intervals permits us to infer that we are dealing with T_6 phase. The Z-direction of G^H (physical reciprocal lattice vector) for $\cos\theta = 1/2$ is given by

$$G_z'' = \frac{1}{t_1} \sqrt{8/15} \left[\sum_{i=1}^5 N_i + 2N_6 \right] \quad (42)$$

Any vector having $N_1 = N_2 = N_3 = N_4 = N_5$ will have G_{xy}'' equal to zero. Thus, first spot along 10-fold (periodic) direction can be indexed as $[11111\bar{2}]$. However, $\sum_1^6 N_i$ is equal to 3. This summation will be brought to -2 by subtracting zero vector $[22222\bar{5}]$ or its integral multiple to above. Hence, first spot along 10-fold may be indexed as $[\bar{1}\bar{1}\bar{1}\bar{1}\bar{1}3]$. This direction is periodic and V_6 can be assigned $[\bar{6}\bar{6}\bar{6}\bar{6}\bar{6}18]$. However, $\sum_1^6 N_i = -12$ and we have

proposed $\sum_1^6 N_i = -2, -1, 0, 1, 2$ for uniqueness. This can be achieved by adding zero vector $[44444\bar{10}]$ to this. Hence, the sixth spot V_6 along 10-fold will be indexed by $[\bar{2}\bar{2}\bar{2}\bar{2}\bar{2}8]$ with $\sum_1^6 N_i = -2$. We note that spot V_1 in D-pattern is at 60° to V_6 . This is the reason why

we have chosen $\cos\theta = 1/2$. This spot can be indexed as $[300000]$. To make this unique, we need to add zero vector $[\bar{2}\bar{2}\bar{2}\bar{2}\bar{2}5]$. Hence, indexing of spot V_1 is $[\bar{1}\bar{2}\bar{2}\bar{2}\bar{2}5]$. The diffraction vector $V_{1,P}$, will not have z-component. We may take out z-component from V_1 and index it by $[\bar{2}\bar{1}\bar{1}\bar{1}\bar{1}1]$. All other spots along P-direction can be indexed by inflation / deflation matrix given by us [23,24]. The indexing of spot V_D would again require absence of z-component. This can be achieved by assigning $[003\bar{3}00]$ to this. The indexing of $V_{D,6}$ can be achieved by adding 6-layer height in $[003\bar{3}00]$. The sextuplet of indices thus becomes $[\bar{2}\bar{2}1\bar{5}\bar{2}8]$. We have listed them in Table 2. As mentioned earlier 10-fold diffraction pattern will contain $V_{1,P}$ and $V_{D,6}$ directions. All other spots can be indexed by inflation and deflation matrix [23,24] as we have indicated while indexing diffraction patterns of IQC. We have mentioned earlier that DQC have four types of phases T_2, T_4, T_6 and T_8 . The indexing of spots of V_D type in P-pattern will accordingly be given by $[00n\bar{n}00]$ for T_{2n} phase. The indexing of V_1 type spot in D-pattern will be given by $[100000]$, $[200000]$, $[\bar{1}\bar{2}\bar{2}\bar{2}\bar{2}5]$ and $[\bar{2}\bar{2}\bar{2}\bar{2}\bar{2}5]$ for T_{2n} phases respectively. For T_6 and T_8 , we have differently looking indices due to uniqueness condition of $\sum_1^6 N_i = 0, \pm 1, \pm 2$.

P-pattern			D-pattern		
Spot designation	Indices	After [23]	Spot designation	Indices	After [23]
V_6	$\bar{2}\bar{2}\bar{2}\bar{2}\bar{2}8$	000003	V_6	$\bar{2}\bar{2}\bar{2}\bar{2}\bar{2}8$	000003
V_D	$003\bar{3}00$	$003\bar{3}00$	V_1	$\bar{1}\bar{2}\bar{2}\bar{2}\bar{2}5$	300000
$V_{D,6}$	$\bar{2}\bar{2}1\bar{5}\bar{2}8$	$003\bar{3}03$	$V_{1,P}$	$\bar{2}\bar{1}\bar{1}\bar{1}\bar{1}1$	$0\bar{3}\bar{3}\bar{3}\bar{3}6$

Table 2. Sextuplets of indices assigned to various spots for decagonal phase (T_6 -6 layer periodicity along 10-fold axis)

5. Conclusions

We have discussed reciprocal lattices of icosahedral and decagonal quasicrystals with the help of projection formalism utilized in higher dimensional structural description of such phases. The necessary mathematical details pertaining to higher dimensional crystallography were understood with the help of one dimensional aperiodic case (cf. section 2). It was also shown that we need expression of physical reciprocal lattice vector for mapping the entire diffraction space and indexing of diffraction spots. Such a viewpoint was extended to a six dimensional cubic lattice for the icosahedral phase (cf. section 3). Having got the expression of physical reciprocal lattice vector we have spelt out necessary steps for indexing of diffraction patterns. We have shown the solution of important spots in terms of sextuplets of indices and given them in a table for the readers. We have put forward our generalized formalism based on 6d orthogonal cell for decagonal phases in section 4 of the chapter. A general expression of zone rule as a dot product of physical reciprocal and direct lattice vectors has been given. Two distinct cases corresponding to decagonal phases having $10/m$ and 10_5 screw axis have been given. We have adopted a six index notation for both these structures. The conditions for uniqueness for them are discussed in terms of the ratio of two lattice parameters of the orthogonal cell. The indexing of important diffracted spots corresponding to two distinct two-fold patterns (P and D patterns) has been accomplished for T_6 phase. We have indicated methods of indexing of diffraction patterns for ten-fold zone. At the end of section 4, we have also given the indices of some of the equivalent diffracted spots expected in other decagonal phases.

6. Annexure A

This note to the readers has been added after the announcement of Nobel Prize to Dan Shechtman in Chemistry (2011) for the discovery of quasicrystals in the rapidly solidified Al-Mn alloys [1]. It is important for all of us to know and understand the path of discovery of a truly seminal nature. We need to recall some of the historical facts in this regard. Steurer and Deloudi [2], while reviewing various aspects of quasicrystals in the silver jubilee year of its first report, quoted the legendary materials scientist John Cahn who later co-authored paper [1]. It is mentioned [2] that when Dan went to NIST, USA for sharing his excitement, Cahn said "Go away, Dany. These are twins and that's not terribly interesting". However, when Cahn got convinced, he led the discovery by defending its tantalizing nature from the front. One may substantiate by remembering the chronological order of the lively debate that has gone on. One may recall that when Linus Pauling put forward twinning models [3, 4] for interpreting icosahedral diffraction patterns, Cahn and Gratias supported Shechtman by taking a firm position [5] about the new state of atomic order in the solid state. At this crucial juncture, a leading role was played by a versatile genius, Mackay [6] who demonstrated that diffraction results reported in [1] cannot be understood in terms of fundamental axiom of conventional 3d-crystallography. It is against this background that Senechal [7] titled the discovery of long range aperiodic order with sharp diffraction patterns [1] as the demise of a paradigm. The demise pertains to foundation of classical 3d crystallography where we get the impression that diffraction patterns cannot display invariance under non-crystallographic point symmetry. The selected area diffraction

patterns that remain invariant under icosahedral point group have given rise to a new paradigm that led to a change in the definition of crystal by International Union of Crystallography in 1992 [2].

The profound impact of the emergence of new paradigm can be understood by going through the foreword by Freeman Dyson [8]. While writing foreword for the book [8] entitled "The Mathematical Century", he remarked discovery of quasicrystals as one of the three jokes of nature of the last century. The other two jokes are (a) appearance of imaginary quantity in the solution of Schrodinger wave equation in quantum mechanics and (b) possible states in quantum mechanics forming a linear space, which have much wider ramification and deeper connection with the fundamental laws of nature governing mechanics of quantum particles. Thus, experimental observation of Quasiperiodic translational order is truly revolutionary and has led to a veritable change in our age old belief of classical crystallography. The paintings in ancient art perhaps inspired generations of mathematicians to systematically develop mathematics for tilings, coverings and packings that are not periodic. In this context, it is important to mention contributions of Penrose [9] and Mackay [10] prior to the discovery of icosahedral quasicrystals. Intellectually stimulating exercises of many such authors helped experimentalists to visualize images of possible underlying atomic arrangements and their Fourier transforms in reciprocal space.

There are many reviews and books summarizing developments in this fascinating area. Some of these are given in this chapter. For Indian contributions, we refer the readers to a report by international union of crystallography [11]. Indian experimental investigations prior to the first report of diffraction patterns with non-crystallographic point group symmetry are seen to have patterns akin to D-patterns of decagonal phases [12]. We are able to recognize this only in retrospect after we have the necessary knowledgebase on quasicrystals. In contrast, Shechtman and his colleagues' perseverance to determine the invariance of diffraction patterns under icosahedral point group symmetry and bold announcement to the scientific community are testimony to the fact that discoverers are genius and courageous men/women of all times. Hence, the discovery being a class of its own for which Shechtman as the chief architect has rightly been chosen for the Nobel Prize.

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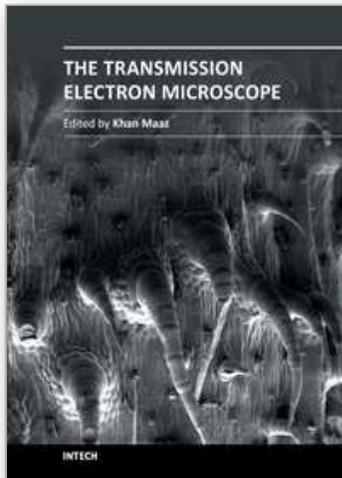
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Edited by Dr. Khan Maaz

ISBN 978-953-51-0450-6

Hard cover, 392 pages

Publisher InTech

Published online 04, April, 2012

Published in print edition April, 2012

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