ties of the dynamic wave field: (i) at resonance, there is a remarkable increase of the total primary beam current near the crystal surface; (ii) the penetration of the wave field below the corresponding beam emergence threshold is rather small.

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# The Octagonal Quasilattice and Electron Diffraction Patterns of the Octagonal Phase 

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#### Abstract

An analysis is given of the dual transformation and also the strip method which can yield the ideal octagonal quasilattice as well as its approximants. An ideal octagonal tiling consisting of $45^{\circ}$ rhombi and squares can be derived from the projection of a 4 D cubic lattice within an irrational 2D subspace onto an irrational 2D hyperplane, and its Fourier transform matches well the eightfold electron diffraction pattern of the $\mathrm{Cr}-\mathrm{Ni}-\mathrm{Si}$ octagonal quasicrystal. The approximant of an octagonal tiling corresponds to the rearrangement of two kinds of tiles in an ideal quasilattice which destroys the exact quasiperiodic sequence. It is shown that the defects introduced to change the aperiodic order into a regular approximant correspond to a linear phason strain along certain directions, and this will break the eightfold rotational symmetry. The Fourier transform agrees well with the experimental electron diffraction pattern displaying only fourfold symmetry.


[^0]
## Introduction

The discovery of a quasicrystal with icosahedral symmetry in an Al-Mn alloy by Shechtman, Blech, Gratias \& Cahn (1984) has initiated much activity in the experimental and theoretical studies of non-crystallographic symmetry of aperiodic crystals (Henley, 1987; Kuo, 1988). Quite recently, the discovery of an octagonal quasicrystal in rapidly solidified $\mathrm{Cr}-\mathrm{Ni}-\mathrm{Si}$ and other alloys has been reported by Wang, Chen \& Kuo (1987). The diffraction patterns of the new structure show a two-dimensional (2D) quasiperiodicity with eightfold rotational symmetry and onedimensional periodicity along the eightfold axis. This is rather similar to the 2D decagonal quasicrystal (Bendersky, 1985). The point group symmetry $D_{8 h}(8 / \mathrm{mmm})$ is incompatible with any periodic lattice and therefore does not occur in crystals. The aperiodic lattice has recently been derived by many methods (Duneau \& Katz, 1985; Elser, 1986; Kramer \& Neri, 1984; Socolar \& Steinhardt, 1986) which are based mainly on de Bruijn's (1981) work on Penrose tilings (Penrose, 1974). In addition, non-crystallographic group theory including the octagonal case
has been developed (Janssen, 1986; Rokhsar, Wright \& Mermin, 1988). Considerations of the octagonal tiling in different approaches have also been advanced (Beenker, 1982; Luck, 1988; Watanabe, Ito \& Soma, 1987).

In real quasicrystals, however, defects exist abundantly as shown by diffuse diffraction spots. A concept which has proved useful in the description of the systematic disorder observed experimentally in aperiodic crystals is that of 'phason strain' (Bak, 1985; Lubensky, Socolar, Steinhardt, Bancel \& Heiney, 1986). The same phason strain can also be introduced in a regular or irregular way in the octagonal quasilattice to change it into an approximant. In most cases, the phason strain is a linear regular change which is manifested by the shift of some peaks away from the positions predicted for exact octagonal symmetry.

The purpose of this paper is to discuss ideal and non-ideal octagonal lattices and their Fourier transforms so as to develop an understanding of the newly discovered octagonal quasicrystal and to interpret the experimentally observed electron diffraction patterns. In § 1 we present a basic overview of the 2D octagonal tiling. § 2 deals with the mathematical analysis of the approximant of the octagonal tiling and an example is given in $\S 3$ to explain the distortions in experimental electron diffraction patterns of some octagonal phases.

## 1. 2D octagonal tiling

Consider the four-dimensional (4D) hypercubic lattice in $E^{4}$. Its point symmetry group is the hyperoctagonal group $\Omega(4)$. The elements of $\Omega(4)$ are four permutations of the symmetry group $S(4)$. For the octagonal case, we have a set of basis vectors which generate a 4D cubic lattice through the relation

$$
\begin{equation*}
\mathrm{e}=Q . \mathrm{I} \tag{1.1}
\end{equation*}
$$

where $I$ is a set of 4D Cartesian basis vectors, and

$$
Q=(1 / \sqrt{ } 2)\left|\begin{array}{cccc}
1 & 0 & 1 & 0  \tag{1.2}\\
1 / \sqrt{2} & 1 / \sqrt{2} & -1 / \sqrt{2} & 1 / \sqrt{2} \\
0 & 1 & 0 & -1 \\
-1 / \sqrt{2} & 1 / \sqrt{2} & 1 / \sqrt{2} & 1 / \sqrt{2}
\end{array}\right| ;
$$

so we have a vector in $E$ which can be written as

$$
\begin{equation*}
\mathbf{r}=\sum_{i=1}^{4} n_{i} \mathbf{e}_{i} \tag{1.3}
\end{equation*}
$$

The set $\Sigma$ of all these vectors is invariant under an eightfold rotation $X$ and a vertical mirror $v$. The two operations generate a group isomorphic with $D_{8}$. If we add a central inversion $\sigma$, then it generates a group isomorphic with $D_{8 h}=D_{8} \times C_{2}$ which is a subgroup of $S(4)$. The action of these three elements on the
basis vectors $\mathbf{e}$ is given by

$$
\begin{gathered}
\Gamma(X)=\left|\begin{array}{rrrr}
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
-1 & 0 & 0 & 0
\end{array}\right| ; \quad \Gamma(v)=\left|\begin{array}{rrrr}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 \\
0 & 0 & -1 & 0 \\
0 & 1 & 0 & 0
\end{array}\right| ; \\
\Gamma(\sigma)=\left|\begin{array}{rrrr}
-1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & -1
\end{array}\right| .
\end{gathered}
$$

Apparently, a 4D space group can be constructed with a 4D translational subgroup based on the holohedral point group $D_{8 h}$. This point group has subgroups $C_{8}, C_{8} \times C_{2}$ and $D_{8}$ that belong to the same 4D Bravais lattice. For each of the corresponding matrix groups one may determine the possible 4D space group (Janssen, 1986). The corresponding 4D lattice is compatible with the 2D octagonal Bravais lattice. From (1.1), the selection of the first two or last two columns of $Q$ determines a projection of the related vectors from $E^{4}$ to two 2D orthogonal spaces $E_{\|}^{2}$ and $E_{\perp}^{2}$, respectively. In $E_{\|}^{2}$ and $E_{\perp}^{2}$, the projected four basis vectors (see Fig. 1) become

$$
\mathbf{e}_{\|}=Q_{\| \|} \cdot \mathbf{I}_{\|} ; \quad \mathbf{e}_{\perp}=Q_{\perp} \cdot \mathbf{I}_{\perp}
$$

and

$$
\begin{align*}
& Q_{\|}=(1 / \sqrt{2})\left|\begin{array}{cc}
1 & 0 \\
1 / \sqrt{2} & 1 / \sqrt{2} \\
0 & 1 \\
-1 / \sqrt{2} & 1 / \sqrt{2}
\end{array}\right| ; \\
& Q_{\perp}=(1 / \sqrt{2})\left|\begin{array}{cc}
1 & 0 \\
-1 / \sqrt{2} & 1 / \sqrt{2} \\
0 & -1 \\
1 / \sqrt{2} & 1 / \sqrt{2}
\end{array}\right| . \tag{1.4}
\end{align*}
$$

It is proved that the reducible 4 D representation of the group $D_{8 \mathrm{~h}}$ can be decomposed orthogonally into two nonequivalent irreducible 2D representations in the two 2D spaces, $E_{\|}^{2}$ and $E_{\perp}^{2}$ respectively. Also, this decomposition is an irrational reducible so that the corresponding projected structure is a 2 D


Fig. 1. Projected basis vectors $\left\{\mathbf{e}_{i}^{1}\right\}$ and $\left\{e_{i}^{e}\right\}$ in $E_{\|}^{2}$ and $E_{1}^{2}$, respectively.
quasiperiodic structure with eightfold symmetry. The 3D structure is a layer structure which has a periodicity along the direction perpendicular to the aperiodic layers.

As is well known, several authors have proposed some variations of the projection method to obtain a quasiperiodic lattice which could reproduce the experimentally observed diffraction patterns. These methods can be grouped into two classes: the direct projection (Duneau \& Katz, 1985; Elser, 1986; Kalugin, Kitaev \& Levitov, 1986) and the dual method (de Bruijn, 1981; Beenker, 1982; Socolar \& Steinhardt, 1986). Dual methods are based on the projection of a higher-dimensional grid into a lowerdimensional space. Each region defined by the projected grid is then associated with a point (dual transformation) or a vertex of the unit-cell packing. In our case, we derive a 2D octagonal tiling by the regular dual grid transformation with $\sum \gamma_{i}=0$ [see Fig. 2; $\gamma_{i}$ is a shift parameter along the $i$ th direction ( $i=1,2,3,4)$ ]. We can see that all properties of an octagonal quasilattice are shown here. Along a bond direction the ratio of the two types of length is $\sqrt{2}$. Owing to similarity, there are plenty of local centres of eightfold symmetry which in turn are arranged with an eightfold symmetry. The basic unit cells are two kinds of tiles: square and $45^{\circ}$ rhombus. Gaehler \& Rhyner (1985) have proved that the tiling space and dual space in the dual transform are equivalent to the lower-dimensional hyperplane and subspace in the direct projection method. Thus, the vertices of the octagonal tiling can also be described in terms of the projection of a 4D lattice within an irrational subspace defined by $Q_{\perp}$ onto a 2D irrational hyperplane defined by $Q_{\|}$, and we can determine the


Fig. 2. An ideal aperiodic octagonal tiling consists of squares and $45^{\circ}$ rhombi.
projection operators $P_{\|}$and $P_{\perp}$ by using the relations

$$
\begin{equation*}
P_{\| \mid} \mathbf{e}=\mathbf{e}_{\|} ; \quad P_{\perp} \mathbf{e}=\mathbf{e}_{\perp} \tag{1.5}
\end{equation*}
$$

and

$$
\begin{aligned}
& P_{\|}=(1 / 2)\left|\begin{array}{cccc}
1 & 1 / \sqrt{2} & 0 & -1 / \sqrt{2} \\
1 / \sqrt{2} & 1 & 1 / \sqrt{2} & 0 \\
0 & 1 / \sqrt{2} & 1 & 1 / \sqrt{2} \\
-1 / \sqrt{2} & 0 & 1 / \sqrt{2} & 1
\end{array}\right| ; \\
& P_{\perp}=(1 / 2)\left|\begin{array}{cccc}
1 & -1 / \sqrt{2} & 0 & 1 / \sqrt{2} \\
-1 / \sqrt{2} & 1 & -1 / \sqrt{2} & 0 \\
0 & -1 / \sqrt{2} & 1 & 1 / \sqrt{2} \\
1 / \sqrt{2} & 0 & -1 / \sqrt{2} & 1
\end{array}\right| .
\end{aligned}
$$

Obviously, $P_{\|}^{2}=P_{\|}, P_{\|} P_{\perp}=\theta$ ( $\theta$ is a matrix with zero elements).

Following the same approach used in the case of crystals, the reciprocal basis $\mathrm{e}^{*}$ of e can readily be constructed according to

$$
\begin{equation*}
\mathbf{e}_{i} \cdot \mathbf{e}_{j}^{*}=\delta_{i j} \tag{1.6}
\end{equation*}
$$

where $\mathrm{e}^{*}=Q^{*} . \mathrm{I}$, and then

$$
\begin{equation*}
Q^{*}=\tilde{Q}^{-1}=Q, \tag{1.7}
\end{equation*}
$$

i.e. the basis $\mathrm{e}^{*}$ of the set in the 4 D reciprocal lattice $\Sigma^{*}$ is the same as that of $\Sigma$. However, it should be mentioned that, unlike crystals, the reciprocal basis $\mathbf{e}^{*}$ now corresponds only to the rotational symmetry of the octagonal phase, and the corresponding quasiperiodicity in real space can be described by the self similarity of the structure. Now let us consider the calculation of the Fourier transform of an octagonal tiling in a simple case of identical atoms occupying all projected points in $E^{4}$. We define a 4D structure factor by

$$
\begin{equation*}
F(\mathbf{g})=\sum_{\mathbf{r} \in \Sigma} f_{\mathbf{r}} \exp (i \mathbf{g} \cdot \mathbf{r}) \tag{1.8}
\end{equation*}
$$

with $\mathbf{g} \in \Sigma^{*}$ and $\mathbf{r} \in \boldsymbol{\Sigma}$. Decomposing the 4D vectors $\mathbf{g}$ and $\mathbf{r}$ into components perpendicular and parallel to the 2D hyperplane, we obtain

$$
\begin{equation*}
\mathbf{r}=\mathbf{r}_{\|}+\mathbf{r}_{\perp} \quad \text { and } \quad \mathbf{g}=\mathbf{g}_{\|}+\mathbf{g}_{\perp}, \tag{1.9}
\end{equation*}
$$

and then the structure factor of an octagonal structure obtained by the projection is

$$
\begin{equation*}
F\left(\mathbf{g}_{\|}\right)=\sum_{\mathbf{r} \in C_{\perp}} f_{\mathbf{r}_{\|}} \exp \left(-i \mathbf{g}_{\perp} \cdot \mathbf{r}_{\perp}\right) \tag{1.10}
\end{equation*}
$$

where $C_{\perp}$ is the projection of a 4 D hypercubic cell $C(\mathbf{n})$ onto $E_{\perp}^{2}$ (see Fig. 3) which can be considered as the window function of $E_{\perp}^{2}$ in the projection method. Suppose $f_{r_{\|}}=1$ and the number of atoms is infinite; then

$$
\begin{equation*}
F\left(\mathbf{g}_{\|}\right)=1 / \mu\left(C_{\perp}\right) \int_{C_{\perp}} \exp \left(-i \mathbf{g}_{\perp} \cdot \mathbf{r}_{\perp}\right) \mathrm{d}^{2} \mathbf{r}_{\perp}, \tag{1.11}
\end{equation*}
$$

Table 1. List of peaks of the octagonal quasilattice having $\left|m_{\|}\right|<7$ and $\left|m_{\perp}\right|<1.6$

The relative intensities are given in the table and the peaks can be indexed by four integers. The serial number corresponds to that of the spots in Fig. 4.

| Label | $m_{1}$ | $m_{2}$ | $m_{3}$ | $m_{4}$ | $I\left(m_{\\|}\right)$ | $\left\|m_{\\|}\right\|$ | $\left\|m_{\perp}\right\|$ |
| :---: | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 0 | 0 | 0 | 0 | 1.000 | 0.000 | 0.000 |
| 1 | 1 | 0 | 0 | 0 | 0.418 | 1.000 | 1.000 |
| 2 | 0 | 1 | 0 | 1 | 0.153 | 1.414 | 1.414 |
| 3 | 1 | 1 | 0 | 0 | 0.607 | 1.848 | 0.765 |
| 4 | 1 | 1 | 0 | 1 | 0.867 | 2.414 | 0.414 |
| 5 | 1 | 1 | 1 | 1 | 0.356 | 2.613 | 1.082 |
| 6 | 1 | 2 | 1 | 0 | 0.750 | 3.414 | 0.586 |
| 7 | 1 | 2 | 1 | 1 | 0.301 | 3.558 | 1.159 |
| 8 | 2 | 2 | 0 | 0 | 0.104 | 3.696 | 1.530 |
| 9 | 1 | 2 | 2 | 0 | 0.647 | 4.182 | 0.717 |
| 10 | 1 | 2 | 2 | 1 | 0.920 | 4.461 | 0.317 |
| 11 | 2 | 2 | 2 | 0 | 0.556 | 4.828 | 0.828 |
| 12 | 1 | 3 | 2 | 1 | 0.476 | 5.398 | 0.926 |
| 13 | 2 | 3 | 2 | 0 | 0.976 | 5.828 | 0.172 |
| 14 | 2 | 3 | 3 | 1 | 0.407 | 5.914 | 1.015 |
| 15 | 1 | 3 | 3 | 1 | 0.846 | 6.309 | 0.449 |
| 16 | 1 | 3 | 3 | 2 | 0.731 | 6.755 | 0.610 |
| 17 | 2 | 4 | 2 | 0 | 0.293 | 6.828 | 1.172 |

so that $I\left(\mathbf{g}_{\|}\right)=\left|F\left(\mathbf{g}_{\|}\right)\right|^{2} . \mu\left(C_{\perp}\right)$ is the area of the corresponding projected cell which is an octagon, as shown in Fig. 3. Then $\mu\left(C_{\perp}\right)=2(1+\sqrt{2})$. The calculated result is given in Table 1. We see that the calculated pattern matches fairly well the experimental one (see Fig. 4), particularly the positions of the spots.

Like other quasicrystals, the diffraction pattern of an octagonal phase can be indexed by using its self similar transformation. As the inflation and deflation factors are respectively (Beenker, 1982)

$$
\begin{equation*}
f=\sqrt{2}+1 \quad \text { and } \quad f^{-1}=\sqrt{2}-1 \tag{1.12}
\end{equation*}
$$

the transformation can be given by a $4 \times 4$ matrix $M$,

$$
M=f P_{\|}-f^{-1} P_{\perp}=\left|\begin{array}{rrrr}
1 & 1 & 0 & -1  \tag{1.13}\\
1 & 1 & 1 & 0 \\
0 & 1 & 1 & 1 \\
-1 & 0 & 1 & 1
\end{array}\right|
$$

The eigenvalue of $M$ is $\sqrt{2}+1$ or $\sqrt{2}-1$. One can check that $M$ commutes with the action of the octagonal group $D_{8 h}$ so that $E_{\|}^{2}$ and $E_{\perp}^{2}$ are still


Fig. 3. The projection of a 4D unit cell onto $E_{\perp}^{2}$ which is an octagon divided into six subcubes.
invariant subspaces. Then all possible peaks in the diffraction pattern have the indices (see Table 1)

$$
\begin{equation*}
m_{i}^{\prime}=\sum_{j=1}^{4} M_{i j} m_{j} \quad(j=1,2,3,4) . \tag{1.14}
\end{equation*}
$$

## 2. Approximants of octagonal tiling

An octagonal tiling consists of two unit cells, and its vertices can be obtained either as duals to the meshes of a regular tetragrid, or by projecting from a 4D simple cubic lattice within an irrational strip in $E^{4}$.

(a)

(b)

Fig. 4. (a) Eightfold electron diffraction pattern in a rapidly solidified $\mathrm{Cr}-\mathrm{Ni}-\mathrm{Si}$ alloy (Wang et al., 1987); (b) simulated diffraction pattern corresponding to Fig. 2. The spots with intensity $I\left(\mathbf{g}_{\|}\right)>0.01$ are plotted (see also Table 1).

In fact, $Q_{\|}$determines the size and shape of unit cells presented in the aperiodic structure and $Q_{\perp}$ the corresponding topology. If the strip is placed at a commensurate orientation, the corresponding structure is a crystal or an approximant of the octagonal tiling. It consists of the same unit cells but their arrangement does not follow the exact matching rules of an ideal octagonal tiling. In other words, it can still be described by the four basis vectors but its symmetry deviates from $D_{8 h}$. The analogous geometry properties have also been studied by many authors (Elser \& Henley, 1985; Yang \& Kuo, 1987). They found that the projection method can derive both quasiperiodic and periodic structures and the quasiperiodic structure can be viewed as the limit of a sequence of periodic approximants.

First, let us consider a 1D aperiodic sequence which consists of a series of long ( $L$ ) and short ( $S$ ) intervals with ratio $\sqrt{2}$ of $L$ and $S$. The sequence has a similarity related to an inflation or deflation factor of $\sqrt{2}+1$ or $\sqrt{2}-1$, so that the sequence can be derived by a transformation (see Lu, Odagaki \& Birman, 1986)

$$
\left|\begin{array}{l}
S^{\prime}  \tag{2.1}\\
L^{\prime}
\end{array}\right|=U\left|\begin{array}{l}
L \\
S
\end{array}\right|
$$

and

$$
U=\left|\begin{array}{ll}
1 & 1  \tag{2.2}\\
1 & 2
\end{array}\right| .
$$

The 1D sequence may be obtained in terms of the projection of a 2D cubic lattice onto a straight line of slope $\sqrt{2}$ in the 1D physical space, to give those lattice points whose projections on the axis perpendicular to this physical line fall within a specified window. The $\sqrt{2}$ aperiodic sequence can be obtained by selecting an irrational strip which includes the lattice points whose projections fall on the irrational physical line. To obtain an approximant of the $\sqrt{2}$ series, one replaces the irrational strip by another one, such as a rational or a random one defined by a singled-value window function. We then get a series of 1 D sequences of the same units that appeared in an aperiodic sequence but with different arrangements, either regular or random.

The rational approximant of $\sqrt{2}$ is a continued fraction expansion $\left\{T_{l}\right\}=\{1,1,2,3,5,7,12,17,29$, $41, \ldots\}$. It can easily be shown that the number of $S$ is $T_{l-1}$ and that of $L$ is $T_{l-2}$ in this $\sqrt{2}$ series, and their ratio is given by $T_{l-1} / T_{l-2}$. This ratio is a rational number since both $T_{l-1}$ and $T_{l-2}$ are integers. The unit cell of the approximant has $T_{l}$ intervals and its size increases with the order of $l$; these two numbers tend to infinity as the ratio $T_{l-2} / T_{l-1}$ becomes closer and closer to $\sqrt{2}$, i.e. the direction of a strip tends to an irrational one. The larger the periodically repeating sequence, the better the approximation. The 1D sequence relating to $\sqrt{2}$ is as follows:

1st: $\quad S L$
2nd: SLSSL
3rd: SLSSLSLSLSSL
4th: SLSSLSLSLSSLSLSSLSLSSLSLSLSSL.
If we take the second-order rational approximant then we have a 1D sequence,

## SLSSLSLSSLSLSSLSLSSLSLSSL

compared with the aperiodic one,

## SLSSLSLSLSSLSLSSLSLSSLSLS.

We find that there are defects introduced by the flip of two units at some places, for example, in the underlined positions. If the flip of these two units takes place randomly in a perfect sequence, then a random approximant can be obtained, for example

SSLSSLSLSLSSSLSLSSLSLSLSSSSLSLSLSSL.


Fig. 5. Possible error arrangements, (a), (b) and (c), in an ideal octagonal tiling. The dual grid and associated local tiling show the variation of topological transformation. Dashed lines denote the local configuration before the variation.

In this case, the strip window function is a random function with a single value.

The above consideration can easily be extended to a 2D octagonal tiling such that a flip is replaced by a local exchange in the arrangement of unit cells. The three basic errors which appear in an ideal octagonal tiling are given in Figs. $5(a),(b)$ and (c). From the variation of dual grid and the associated local tiling, we see that the deviation of $Q_{\perp}$ results only in topological changes between adjacent tiles in a perfect structure. The 2D coordinate of each point in the plane, $\mathbf{r}_{\|}$, can be supplemented by another 2D coordinate, $r_{\perp}$, such that the combination $r_{\|}+r_{\perp}$ is a lattice point in 4D space. The orthogonal supplement may be thought of as an order parameter of the structure which can be expressed by four integers as $n_{1} a_{1}+\ldots+$ $n_{4} a_{4}$. The line defect can be applied to this definition by introducing a linear variation along some direction, i.e. $\mathbf{r}_{\perp}^{\prime}=\mathbf{r}_{\perp}+\Delta \mathbf{r}_{\perp}$ and $\Delta \mathbf{r}_{\perp}\left(\mathbf{r}_{\|}\right) \propto \mathbf{r}_{\|}$. By the same reasoning, a random defect corresponds to a random


Fig. 6. (a) A random approximant. There are many local configurations disallowed in an ideal octagonal tiling which destroy the exact $\sqrt{2}$ quasiperiodic sequence of the structure. (b) A periodic approximant of an octagonal tiling which can be constructed approximately by a large unit cell defined by the dashed square.
fluctuation $\Delta \mathbf{r}_{\perp}\left(\mathbf{r}_{\|}\right)$with a zero statistical average. In this paper, we show two typical approximants: one random (Fig. 6a) and the other regular (Fig. 6b). The defects introduced here have a broken continuous symmetry not present in a regular periodic structure. In a sufficiently large region, random defects existing in a random approximant lead to peak broadening in the diffraction pattern and linear ones existing in a regular approximant lead mainly to peak shifts. The latter phenomenon has been found in experiments and we will give a brief consideration in $\S 3$.

Socolar, Lubensky \& Steinhardt (1986) have shown that local-exchange errors of unit cells in a quasilattice can be associated with variation in phase in the density-wave description of the quasicrystal. Such rearrangements leading to phase shifts have been called phasons in incommensurate systems (Bak, 1982).

## 3. An example of a $\mathbf{3 / 2}$ approximant

In general, the approximant of an octagonal tiling consists of almost periodically repeated 'aperiodic' blocks. For a simple case, the approximant is obtained by the dual transform when $\sqrt{2}$ in $Q_{\perp}$ [see (1.4)] is approximated by $3 / 2$. Note that their mismatches are considered as linear phason strains. Also, in this case one can show that the set of maxima in the diffraction pattern coincides with the projection of the 4D reciprocal lattice. According to (1.5), if

$$
Q=(1 / \sqrt{2})\left|\begin{array}{cccc}
1 & 0 & 1 & 0  \tag{3.1}\\
1 / \sqrt{2} & 1 / \sqrt{2} & -2 / 3 & 2 / 3 \\
0 & 1 & 0 & -1 \\
1 / \sqrt{2} & 1 / \sqrt{2} & 2 / 3 & 2 / 3
\end{array}\right|
$$

then

$$
Q^{*}=[\sqrt{2} /(1+\sqrt{8} / 3)]\left|\begin{array}{cccc}
\sqrt{8} / 3 & 0 & 1 & 0  \tag{3.2}\\
1 / \sqrt{2} & 1 / \sqrt{2} & -1 / \sqrt{2} & 1 / \sqrt{2} \\
0 & \sqrt{8} / 3 & 0 & -1 \\
-1 / \sqrt{2} & 1 / \sqrt{2} & 1 / \sqrt{2} & 1 / \sqrt{2}
\end{array}\right| .
$$

From § 1 we know that $Q$ determines the order in a real structure and the relative intensity in the corresponding Fourier spectrum. Thus, (3.1) and (3.2) show that with the linear variation of topological order (related to $Q_{\perp}$ ) in real space there will be peak shifts (related to $Q^{*}$ ) in the reciprocal space along certain directions. In our example, along the two directions at 45 and $135^{\circ}$ the ratio of the basis vector lengths is about $\sqrt{8} / 3$. Furthermore, both the real structure and its Fourier transform derived by the projection method show that there is a departure from or breaking of the eightfold symmetry. For this approximant, the structure consists approximately of quite large unit cells (one of them is outlined by
dashed lines in Fig. 6b), and the anisotropy in reciprocal space apparently appears in the two directions at 45 and $135^{\circ}$ denoted by arrows in Fig. 7(b). The line defects introduced in the structure lead to the corresponding peak shifts in the Fourier transform. The weak spots close to the centre in these directions tend approximately to a periodic distribu-

(a)

(b)

Fig. 7. (a) Electron diffraction pattern of a rapidly solidified Mn-$\mathrm{Fe}-\mathrm{Si}$ alloy with a broken eightfold symmetry. The weak spots along the 45 and $135^{\circ}$ directions are more or less periodic, as shown by the arrow heads (Zhou, 1987). (b) The Fourier transform of the structure shown in Fig. 6(b). Along the directions indicated by arrows the weak spots close to the centre tend to distribute periodically with a pseudo-fourfold symmetry.
tion displaying a pseudo-fourfold symmetry (marked by arrowheads in Fig. 7b). As mentioned before (Lubensky, Socolar, Steinhardt, Bancel \& Heiney, 1986), the lower the intensity, the greater the peak shift; this means the shift is proportional to $\left|\mathbf{g}_{\perp}\right|$ for linear phasons. Such a peak shift has in fact been observed in the electron diffraction pattern (Fig. 7a) of a new octagonal quasicrystal in an $\mathrm{Mn}-\mathrm{Fe}-\mathrm{Si}$ alloy (Zhou, 1987). This implies that this quasicrystal was grown under anisotropic stresses during rapid solidification. Wang \& Kuo (1987) have shown that on heating to 670 K this pseudo-fourfold symmetry gradually changed to an eightfold one, implying stress relaxation and a gradual disappearance of defects.

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