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A COMPARATIVE STUDY OF ZONE AXIS PATTERN MAPS FROM DECAGONAL PHASES WITH VARYING PERIODICITY

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Introduction

The discovery in 1985 of the decagonal phase with periodicity in one direction and quasiperiodicity in the other two directions has excited considerable interest (1,2). This was followed by the observation that the periodicity perpendicular to the quasiperiodic plane can assume multiple values of n=[1,2,3,4]x0.4 nm (3,4). The mapping of reciprocal spaces of these phases, labelled T_{2n}, by electron diffraction is important in the context of atomic models for the decagonal phase. While partial determinations have been available for T_4 [Al-Co] (5), T_6 [Al-Mn] (6-8) and T_8 [Al-Fe] (9), [Al-Pd] (10,11), the recent complete determination of zone axis pattern maps [ZAPM] and Kikuchi maps of T_6 [Al-Mn] with 1.24 nm periodicity (12) and T_4 [Al-Cu-Co-Si] with 0.8 nm periodicity is a tour de force by Kelton and his co-workers (13). These papers coupled with the complete mapping of the HOLZ line (14) and Kikuchi line (15) patterns of the T_2 [Al-Co-Ni] with 0.4 nm periodicity permit us to put in perspective the ZAPM of all the four decagonal phases and in addition predict patterns for the T_8 phase for which a complete experimental determination is still lacking.

Methodology

In arriving at the ZAPM, we follow the strategy adopted by Thangaraj et al.(6). The intense spots in the prominent diffraction patterns are identified (Table 1). In the case of the decagonal phase there are three prominent patterns exhibiting ten fold, two fold and two fold rotational symmetries respectively. The great circles corresponding to the prominent relvectors in these patterns intersect to give the positions of other diffraction patterns. From the intersection we can also determine the corresponding zone axes. Figure 1(a,b) gives the two fold symmetry axis patterns from T_4 and T_6 and identifies the important relvectors. The availability of patterns from reference 13 allows us the correct determination for T_4, whereas the earlier determination (5) was not accurate due to the availability of too few patterns. Figure 2(a,b) gives the stereograms generated by the intersection of the great circles corresponding to the vectors identified in Figure 1. For indexing we have followed the planar pentagonal axes (a1) with the decagonal (c) axis perpendicular to it. While the c/a ratio could assume any value, the observed relationship between the icosahedral and

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decagonal phases dictate a value close to τ^3, if a specific angular relationship is preserved for T_2. c/a values for the other periodicities are corresponding multiples. The zone axes are calculated by a method first advanced by Fitzgerald et al.(7). The angular relationship between zone axes are also calculated by spherical trigonometry. For this, the angle made by a given vector with the decagonal axis was calculated and then the intersection of the trace of this vector with the V2 vector traces was determined on the stereogram to obtain the positions of the zone axes. The zone axes calculated by the indices and spherical trigonometry are listed in Tables 2 and 3 for T_4 and T_6. A comparison with experimentally determined values for T_4 Al-Co (5,16) and Al-Cu-Co-Si (13) and T_6 Al-Mn (8,12) shows excellent agreement with the calculated ones.

TABLE 1

Important Relvectors for Decagonal Phases with Different Periodicities

Phase	Examples	V3	V4	V5
T_2	Al-Co-Ni	$000\bar{1}03$	$000\bar{1}01$	-
T_4	Al-Co-Cu	$000\bar{1}06$	$000\bar{1}02$	-
T_6	Al-Mn	$00\bar{1}0\bar{1}5$	$000\bar{1}03$	$000\bar{1}02$
T_8	Al-Pd	$00\bar{1}0\bar{1}7$	$000\bar{1}04$	$000\bar{1}03$

TABLE 2

Angular Separation from the Decagonal Vector for Different Zone Axes for T4 Decagonal Phase: Calculated values are for c/a=8.472

(a) Zone axes created by V4 $000\bar{1}02$

Zone axis	Indices	Calculation (indices)	Calculation (spherical trigonometry)	Experiment (Kikuchi) (Ref.13)	Experiment (ZAPM) (Ref.5,16)
J	$8\ \overline{21}\ \overline{21}\ 8\ 26\ 4$	62.4	62.4	62.3	62
D	$2\ \bar{2}\ \bar{3}\ 0\ 3\ 1$	43.6	45.1	44.1	45
M	$3\ \bar{8}\ \bar{8}\ 3\ 10\ 4$	36.2	36.1	35.2	36
C	$5\ \bar{5}\ \bar{8}\ 0\ 8\ 4$	31.9	31.8	31.1	32
N	$5\ \overline{13}\ \overline{13}\ 5\ 16\ 8$	30.6	30.5	29.8	-

(b) Zone axes created by V3 $000\bar{1}06$

Zone axis	Indices	Calculation (indices)	Calculation (spherical trigonometry)	Experiment (Kikuchi) (Ref.13)	Experiment (ZAPM) (Ref.5,16)
I	$6\ \overline{16}\ \overline{16}\ 6\ 20\ 1$	80.3	80.1	80.8	80
F	$6\ \bar{6}\ \overline{10}\ 0\ 10\ 1$	72.0	71.6	71.4	72
J'	$2\ \bar{6}\ \bar{6}\ 2\ 8\ 1$	65.9	65.4	66.0	-
E	$4\ \bar{4}\ \bar{6}\ 0\ 6\ 1$	62.3	61.8	61.7	62
K	$2\ \bar{5}\ \bar{5}\ 2\ 6\ 1$	61.1	60.5	60.1	-

Results

The procedure adopted by us allows to identify zone axes, which are exactly parallel and discriminate between those which are nearly parallel. Figure 1 indicates that $(000\bar{1}02)$ of T_4 and $(000\bar{1}03)$ of T_6 are identical in their spatial orientations and hence the zone axes developed by their intersections with the main great circles will be identical. In practice the zone axes developed by $(000\bar{1}03)$ are for a slightly different c/a value. Thus if values from Table 2 and 3 are compared, exact correspondence between the angular values is not achieved. However the difference is very small. By giving the zone axes for T_6 different values so as to make the primary relvectors identical, exact correspondence can be achieved. However, this makes the indices assume rather large numerical values. For T_2, T_4 and T_8 this problem is not encountered and exact correspondence is achieved. The $(000\bar{1}03)$ of T_2 and $(000\bar{1}06)$ of T_4 are also identical in their spatial orientations. Therefore the relationship between zone axes in the T_2 and T_4 will be identical. For this reason the interzonal angles given by Yan et al.(15) for T_2 are close to those given for T_4 in Table 2.

TABLE 3

Angular separation from the decagonal vector for different zone axes for T6 decagonal phase:
Calculated values for c/a=12.708
(a) Zone axes created by V4 $000\bar{1}03$

Zone axis	Indices	Calculation (indices)	Calculation (spherical trigonometry)	Experiment (Kikuchi) (Ref.12)	Experiment (ZAPM) (Ref.8)
J	$3\ \bar{8}\ \bar{8}\ 3\ 10\ 1$	62.9	62.4	64.0	62
D	$3\ \bar{3}\ \bar{5}\ 0\ 5\ 1$	45.7	45.1	45.6	-
M	$1\ \bar{3}\ \bar{3}\ 1\ 4\ 1$	36.7	36.1	37.0	36
C	$2\ \bar{2}\ \bar{3}\ 0\ 3\ 1$	32.4	31.8	31.8	-
N	$2\ \bar{5}\ \bar{5}\ 2\ 6\ 2$	31.1	30.5	31.7	31

(b) Zone axes created by V3 $00\bar{1}0\bar{1}5$

Zone axis	Indices	Calculation (indices)	Calculation (spherical trigonometry)	Experiment (Kikuchi) (Ref.12)	Experiment (ZAPM) (Ref.8)
I	$8\ \overline{21}\ \overline{21}\ 8\ 26\ 1$	78.9	79.0	80.3	79
F	$8\ \bar{8}\ \overline{13}\ 0\ 13\ 1$	69.6	69.7	70.5	-
J	$3\ \bar{8}\ \bar{8}\ 3\ 10\ 1$	62.9	63.0	64.0	62
E	$5\ \bar{5}\ \bar{8}\ 0\ 8\ 1$	58.9	59.1	59.4	-
K	$5\ \overline{13}\ \overline{13}\ 5\ 16\ 2$	57.6	57.9	58.8	-

(c) Zone axes created by V5 $000\bar{1}02$

Zone axis	Indices	Calculation (indices)	Calculation (spherical trigonometry)	Experiment (Kikuchi) (Ref.12)	Experiment (ZAPM) (Ref.8)
L	$8\ \overline{21}\ \overline{21}\ 8\ 26\ 4$	51.9	51.8	52.8	52
C	$2\ \bar{2}\ \bar{3}\ 0\ 3\ 1$	32.4	33.8	31.8	-
O	$3\ \bar{8}\ \bar{8}\ 3\ 10\ 4$	26.0	25.9	26.1	27
B	$5\ \bar{5}\ \bar{8}\ 0\ 8\ 4$	22.5	22.5	21.7	-
P	$5\ \overline{13}\ \overline{13}\ 5\ 16\ 8$	21.5	21.5	21.7	22

It is also clear from Figure 1 that $(000\bar{1}06)$ of T_4 and $(00\bar{1}0\bar{1}5)$ of T_6 are close to each other in spatial orientation. Thus the zone axes generated by their great circles are also close to each other. This is reflected in Tables 2 and 3, where the angular values are comparable. This correlation was also noted by Daulton and Kelton (13).

It is also evident from Figure 1 that $(000\bar{1}02)$ of T_6 has no analogous direction T_4. This is true, even though $(000\bar{1}02)$ exists as a relvector in T_4. Their spatial orientations are vastly different. Atomic models based on this matching must take this factor into account (12).

Our method brings out several additional features for comparison. These points as well as the predicted ZAPM for T_8 will be published elsewhere (17).

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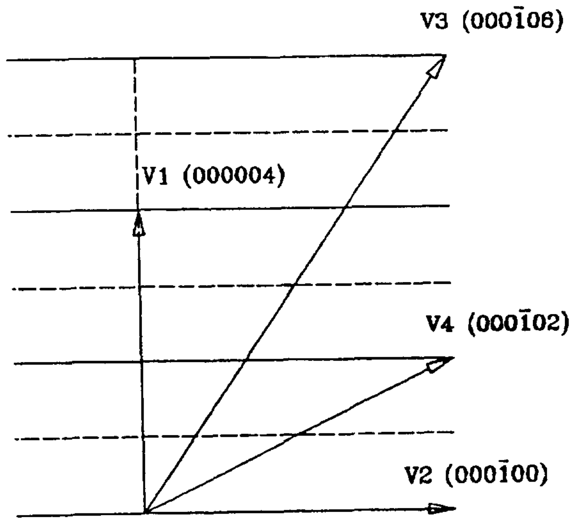

Figure 1(a): The identification of important relvectors V1, V2, V3 and V4 by inspection of the 2-fold pattern of T_4 decagonal phase.

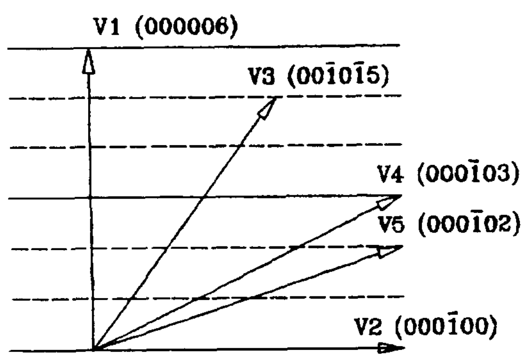

Figure 1(b): The identification of important relvectors V1, V2, V3, V4 and V5 by inspection of the 2-fold pattern of T_6 decagonal phase.

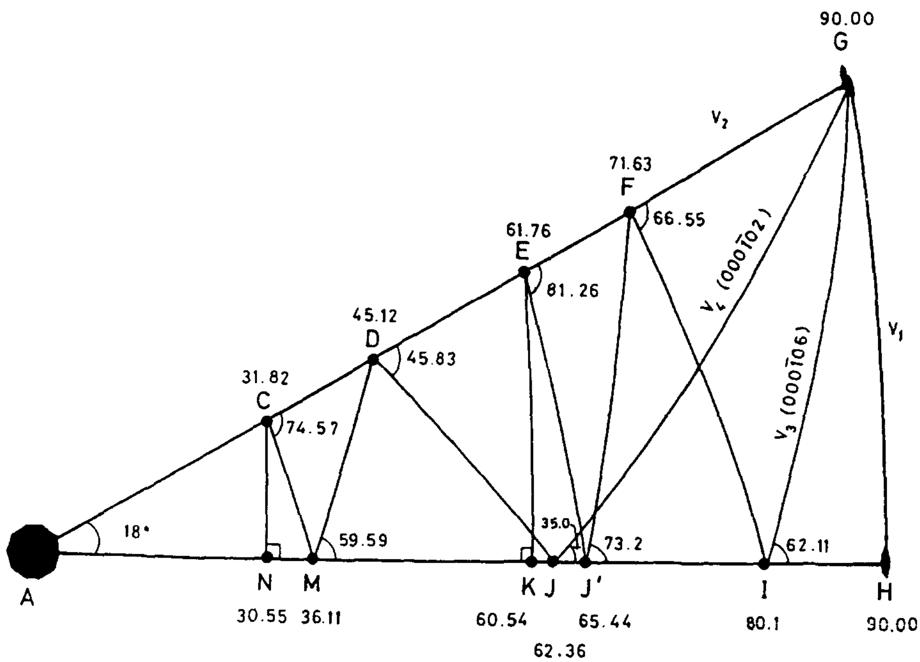

Figure 2(a): Stereogram indicating the traces of great circles corresponding to vectors V1 to V5 for the T_4 decagonal phase. The angular relationships shown are from spherical trigonometric calculations. The vertical axis is expanded by about a factor of two.

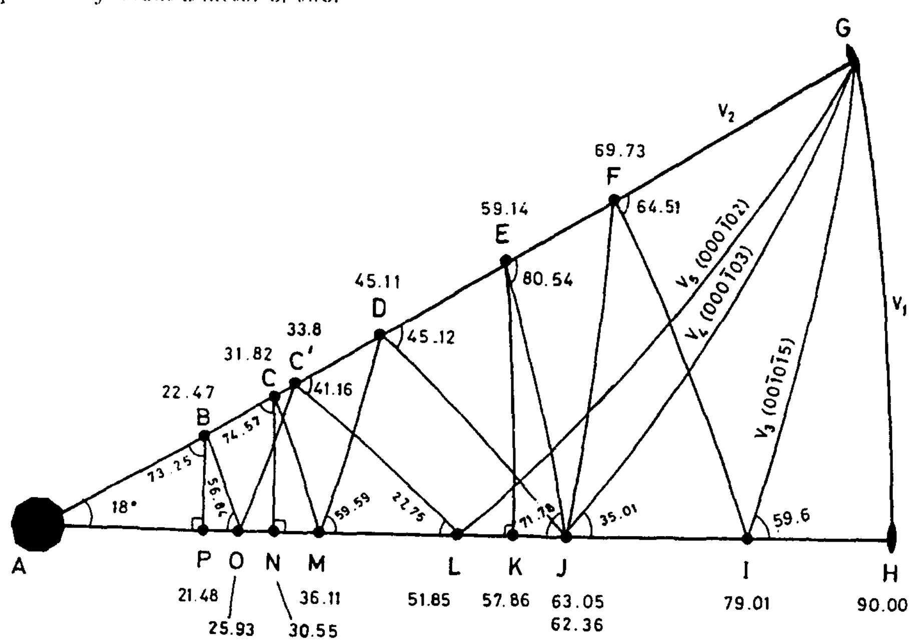

Figure 2(b): Stereogram indicating the traces of great circles corresponding to vectors V1 to V6 for the T_6 decagonal phase. The angular relationships shown are from spherical trigonometric calculations. The vertical axis is expanded by about a factor of two.