Symmetry and Phase Transitions in Decagonal Quasi-Crystals

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ABSTRACT

The possible non-crystallographic point group of the decagonal quasi-crystal phase of Al-Mn alloys has been shown by Bendersky to be either C_{10h} or D_{10h}. For the physically irreducible representations of these groups, we derive the extended integrity basis, Clebsch-Gordan products, stability spaces, and tensorial covariants. The point groups which can arise in phase transitions are determined. It is shown that equilibrium tensorial properties whose components transform as the components of the electrogyration or electrostriction tensors can distinguish between the C_{10h} and D_{10h} point group symmetry of the decagonal phase.

The decagonal or T-phase quasi-crystal is a quasi-crystal with one-dimensional translational symmetry and ten-fold rotational symmetry. Bendersky has shown[1,2] that the non-crystallographic point group symmetry of this quasi-crystal is either C_{10h}(10/m) or D_{10h}(10/mmm). We examine here the group theoretical properties of the physically irreducible representations (PIR) of the point groups C_{10h} and D_{10h} and their implications on phase transitions and tensorial properties of quasi-crystals with such point group symmetries.

The physically irreducible representations (PIR) of the point groups D_{10} and C_{10} are given in Table 1. The irreducible representations of D_{10} are PIRs and denoted by D_i, i=1,2,...,8. The PIRs of C_{10} are denoted by

D_i,i=1,2,5,6,7,8. This nonstandard indexing has been chosen to explicitly show the relationship between the PIRs of C_{10} and D_{10}: The PIRs D_i, i=5,6,7,8 of the point group D_{10} subduced onto the point group C_{10} are the PIRs D_i, i=5,6,7,8. The PIRs of $C_{10h}=C_{10} \times \bar{1}$ and $D_{10h} = D_{10} \times \bar{1}$ are denoted, as is customary, by the symbols D_i^+ and D_i^-, i=1,2,...,8.

For the PIRs of the point groups C_{10h} and D_{10h} we have derived the Clebsch-Gordan products[3], extended integrity basis[4-6] and stability spaces.[7] These tables are published elsewhere.[8]

Central to the application of group theoretical criteria[9-12] to determine the possible symmetries which can arise via a phase transition is the calculation of subduction frequencies. These subduction frequencies are the dimensions of the stability spaces of the PIRs with respect to subgroups of D_{10h} and C_{10h}, and consequently are determined from the tables of stability spaces.

In Table 2 we list for each PIR of C_{10h} and D_{10h} those subgroups which satisfy the chain subduction criterion.[9-12] These are the possible symmetries which can arise via a phase transition where the transition order parameters transform as basis functions of the corresponding PIR. We have also determined that all PIRs of C_{10h} and D_{10h}, except the identity representation, satisfy the Landau stability criterion,and all PIRs satisfy the Lifshitz homogeneity criterion for phase transitions.[9,13]

We have also derived the tensorial covariants for a wide variety of tensors and the PIRs of the point groups C_{10h} and D_{10h}.[8,14,15] We have found that only two types of tensors among those considered are such that their equilibrium form can distinguish between the point groups C_{10h} and D_{10h}. These are tensors which transform as the electrogyration and electrostriction effect tensors.

Gyration G is the magnitude of rotation of the plane c polarization when a plane polarized beam moves through a crystal:[16]

$$G = g_{ij}l_i l_j + A_{k(ij)}E_k l_i l_j$$

where i,j,k = 1,2,3, $\vec{E}$ is an electric field and $\vec{l}$ the distance transversed through the crystal. The gyration tensor g vanishes for both point groups C_{10h} and D_{10h}, and A is the electrogyration tensor.

For D_{10h} we have

$$G = 2A_{x(yz)}[E_x l_y l_z - E_y l_x l_z]$$

and for C_{10h}:

$$G = 2A_{x(yz)}[E_x l_y l_z - E_y l_x l_z] + $$
$$+ 2A_{x(xz)}[E_x l_x l_z - E_y l_y l_z] + $$
$$+ A_{z(xx)}[E_z l_x^2 + E_z l_y^2] + A_{z(zz)}E_z l_z^2$$

The experimental determination of, e.g. the $A_{z(zz)}$ component of the electrogyration tensor can determine which of the two point groups, C_{10h} or D_{10h}, is the point group of the decagonal T-phase quasi-crystal studied by Bendersky.[1,2]

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	Point Group D_{10}		Point Group C_{10}
	C_{10}	C_{2x}	C_{10}
D_1	1	1	1
D_2	1	-1	-1
D_3	-1	1	
D_4	-1	-1	
D_5	$\begin{pmatrix} a^2 & \\ & a^{-2} \end{pmatrix}$	$\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$	$\begin{pmatrix} a^2 & \\ & a^2 \end{pmatrix}$
D_6	$\begin{pmatrix} a^4 & \\ & a^{-4} \end{pmatrix}$	$\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$	$\begin{pmatrix} a^4 & \\ & a^{-4} \end{pmatrix}$
D_7	$\begin{pmatrix} a & \\ & a^{-1} \end{pmatrix}$	$\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$	$\begin{pmatrix} a & \\ & a^{-1} \end{pmatrix}$
D_8	$\begin{pmatrix} a^3 & \\ & a^{-3} \end{pmatrix}$	$\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$	$\begin{pmatrix} a^3 & \\ & a^{-3} \end{pmatrix}$

Table 1: Matrices of generators of the physically irreducible representation (PIR) of the point groups D_{10} and C_{10}. $a = e^{2\pi i/10}$

D_{10h}		C_{10h}	
1+	D_{10h}	1+	C_{10h}
2+	C_{10h}	2+	C_{5i}
3+	$D_{5d}^{(x)}$		
4+	$D_{5d}^{(y)}$		
5+	$D_{2h}^{(j)}$, $C_{2h}^{(j)}$	5+	C_{2h}
6+	$D_{2h}^{(j)}$, $C_{2h}^{(j)}$	6+	C_{2h}
7+	$C_{2h}^{(xj)}$, $C_{2h}^{(yj)}$, C_i	7+	C_i
8+	$C_{2h}^{(xj)}$, $C_{2h}^{(yj)}$, C_i	8+	C_i
1-	D_{10}	1-	C_{10}
2-	C_{10v}	2-	C_{5h}
3-	$D_{5h}^{(x)}$		
4-	$D_{5h}^{(y)}$		
5-	$C_{2v}^{(j)}$, C_2	5-	C_2
6-	$C_{2v}^{(j)}$, C_2	6-	C_2
7-	$C_{2v}^{(xj)}$, $C_{2v}^{(yj)}$, C_s	7-	C_s
8-	$C_{2v}^{(xj)}$, $C_{2v}^{(xj)}$, C_s	8-	C_s

Table 2: For each PIR of the point groups C_{10h} and D_{10h} we list those subgroups which satisfy the chain subduction criterion.

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