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COLOR GROUPS, LANDAU PHASE TRANSITIONS, AND POSSIBLE SPECIES OF FERROIC CRYSTALS

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Abstract— The theory of crystallographic color groups is shown to provide information which simplifies determining the irreducible representations which satisfy the criteria of the Landau theory of continuous phase transitions and in determining the possible species of nonmagnetic ferroic crystals.

INTRODUCTION: COLOR GROUPS

Generalizations of the classical crystallographic groups have been named color groups[1,2]. The elements of color groups consist of elements of classical crystallographic groups combined with some additional operator. A general theory of crystallographic color groups has been given by Koptsik and Kotzev[1] and has been the topic of some recent reviews[3,4]. Well known special cases of color groups are magnetic groups[5], and spin groups[6-10]. These and other color groups have been used in the classification of spin arrangements[5], of crystals with defects[2], and incommensurate crystals[11,12]. We consider here the so-called P-type permutational crystallographic color groups[1]. Permutational color groups are color groups where each element g of a crystallographic group G is combined with a single permutation p of a permutation group P. All permutational color groups can be derived using a method given by van der Waerden and Burckhardt[13]: For each group G and subgroup H' of G one constructs a permutational color group, denoted by G(H'), by combining with each element g the permutation of the left cosets g_iH of G under the action of the element g of G.

There is no general agreement on the definition of equivalence classes of these groups[4]. We have used a definition of equivalence[1,3] chosen on the basis of physical applications of these groups and tabulated[14] all permutational color point groups. Because of our choice of definition of equivalence, the number of such groups is greater than that tabulated by others[1,15,16]. In Table I we list those permutational color point groups G(H') with G=0 (432).

The application of permutational color groups to the Landau theory of continuous phase transitions is via the irreducible representations contained in the representation $D_G^{H'}$ associated with each permutational color group G(H'). The representation $D_G^{H'}$ is the transitive permutation representation of G on the subgroup H' generated by the permutations p combined with each element g in the permutational color group G(H')[14]. In general, the representation $D_G^{H'}$ is reducible into a sum of irreducible representations of the group G. The irreducible representations contained in $D_G^{H'}$ have been tabulated for all permutational color point groups[14]. In Table I we have listed the number of times each irreducible representation of G is contained in $D_G^{H'}$ for each of the permutational color point groups G(H') with G=0.

TABLE I

	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Specie
$O(C_1)$	1	1	2	3*	3*	F
$O(C_2^Z)$	1	1	2	1	1	P
$O(C_2^{XY})$	1		1	1*	2*	F
$O(C_3)$	1	1		1*	1	F
$O(D_2^{(Z,XY,\bar{X}Y)})$	1		1		1*	
$O(C_4)$	1		1	1*		F
$O(D_3)$	1				1*	
$O(D_2^{(Z,X,Y)})$	1	1	2*			
$O(D_4)$	1		1*			
$O(T)$	1	1*				
$O(O)$	1*					

LANDAU THEORY

The Landau theory of continuous phase transitions[17] can be applied to transitions in a crystal between phase of symmetry G and H', a subgroup of G. The density function of the crystal in the low symmetry phase is written as $\rho_1(r)= \rho_o(r) + \Sigma C_m^J \Psi_m^J(r)$ where ρ_o is the density function of the high symmetry phase and the functions $\Psi_m^J(r)$ ar basis functions of irreducible representations D_G^J of the high symmetry phase. For a given high symmetry G and continuous phase transition associated with a specific irreducible representation D_G^J, the lower symmetry H' is found by minimizing the thermodynamic potential $\phi(p,T,C_m^J)$ of the crystal, where p is pressure and T temperature, with the coefficients C_m^J, for the specific J, as variational parameters. Thi minimization determines the density function, above equation, and subsequently the symmetry of the low symmetry phase.

Several group theoretical criteria have been introduced[17-21] which limit the possible symmetries of the low symmetry phase which can arise in a continuous phase transition. These criteria can be reformulated[14] on the basis of the theory of permutational color groups and the representations associated with these groups. Some of these criteria are discussed below.

1. Landau Subgroup Criterion: The group H' is a subgroup of the group G. All subgroups can be found in a tabulation of the permutational color groups G(H'). A complete list of all permutational color point groups is given in reference (14), those with G=0 in Table I. A partial list of permutational color space groups has been published[15,22,23]

2. Subduction Criterion[18]: The irreducible representation D_G^J associated with a continuous phase transition between phases of symmetry G and H' must be such that D_G^J restricted to the subgroup H' contains the identity representation of H'. This criterion can be reformulated as follows[14,24]. The irreducible representation D_G^J associated with a continuous phase transition between phases of symmetry G and H' must be contained in the representation $D_G^{H'}$ associated with the permutational color group G(H'). The irreducible representations contained in $D_G^{H'}$ associated with all permutational color point groups have been tabulated[14], for those groups G(H') with G=0 in Table I. Reading across this table, for example, the row alongside G(H') = $O(C_3)$, one finds that the irreducible representations $D_G^J = \Gamma_1, \Gamma_2, \Gamma_4$, and Γ_5, satisfy the subduction criterion for continuous phase transitions between G=0 and H'= C_3. Reading down the table, for example the column under $D_G^J=\Gamma_3$, one finds that this irreducible representation satisfies the subduction criterion for continuous phase transitions between G=0 and $H'=C_1, C_2^Z, C_2^{XY}, D_2^{(Z,XY,\bar{X}Y)}$, $D_2^{(Z,X,Y)}$, C_4, and D_4. Such tables can also be used in the case of equitranslational phase transitions[14].

3. Chain Subduction Criterion[19,20]: The chain subduction criterion further limits the continuous phase transitions associated with an irreducible representation D_G^J. A continuous phase transition associated with D_G^J which satisfies the subduction criterion

for a transition between G and H' may in fact give rise to a phase transition not to H' but to a larger subgroup of G. The chain subduction criterion takes this into account. The phase transitions which satisfy the chain subduction criterion are found in the tables of the irreducible representations contained in $D_G^{H'}$ [14] (Table I) and are marked with an asterisk. Reading across Table I, for example the row alongside $G(H')=O(C_3)$ one finds that only the irreducible representation $D_G^J=\Gamma_4$ satisfies the chain subduction criterion for phase transitions between G=O and $H'=C_3$. Reading down Table I, for example the column under $D_G^J=\Gamma_3$, one finds that Γ_3 satisfies the chain subduction criterion only for the transitions between G=O and $H'=D_4$ and $D_2^{(Z,X,Y)}$.

The low symmetry groups H' which arise in a continuous phase transition associated with an irreducible representation which satisfies the chain subduction criterion[14] coincide, in the case of point groups, with the tabulation given by Janovec, Dvorak and Petzelt[25] and for equitranslational phase transitions with the tabulation of "Maximum Epikernals" of Asher[25].

4. Tensor Field Criterion[18]: A phase transition in a crystal is a result of a change in some physical property of the crystal. If the physical property is defined by a tensor on the atoms of the crystal, then the tensor field criterion states that the irreducible representation D_G^J associated with the phase transition between G and H' must be contained in the tensor field representation D_G^{TF}: $D_G^{TF}=D_G^T \times D_G^{PERM}$. D_G^T is the representation of the physical property tensor and D_G^{PERM} the permutation representation which describes how the atoms permute under elements of G[15].

It has been shown that the representations D_G^{PERM} are related to the representation $D_G^{H'}$ associated with permutational color groups $G(H')$[14]. For example, if G is the point group of the crystal and H' the site point group of one of the atoms, then the $\vec{k}=0$ irreducible representations contained in the permutation representation are the irreducible representations contained in $D_G^{H'}$ associated with the permutational color point group G(H'). Tables of the irreducible representations D_G^J contained in the second equation, above, for tensor representations $D_G^T = D_G^V$, the polar vector representation, D_G^A, the axial vector representation, $D_G^V \times D_G^A$, and $[D_G^V]^2$, and $D_G^{PERM} \equiv D_G^{H'}$ for all permutational color point groups G(H') have been tabulated[27]. Table II lists such a tabulation for the group G(H') = O(O). Additional physical applications of these tables are considered elsewhere[27].

TABLE II

	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5
$D_G^{H'}$	1				
$D_G^V \times D_G^{H'}$				1	
$D_G^A \times D_G^{H'}$				1	
$(D_G^V \times D_G^A) \times D_G^{H'}$	1		1	1	1
$[D_G^V]^2 \times D_G^{H'}$	1		1		1

POSSIBLE SPECIES OF NONMAGNETIC FERROIC CRYSTALS

The possible species of nonmagnetic ferroic crystals[28] can be determined from the tables of irreducible representations contained in the representation $D_G^{H'}$ associated with the permutational color point groups G(H'). Consider a phase transition between a prototypic phase of prototypic point group symmetry G and a ferroic phase with H' as the ferroic point group of one of the orientation states. Let the orientation state be characterized by a physical property tensor which transforms under G, in the simplest case, as a single irreducible representation D_G^S. Full or partial ferroic species GFH' are determined by the chain-subduction criterion as follows: (1) If the irreducible representation D_G^S is contained in $D_G^{H'}$, and the number of times appears with an asterisk, GFH' is a full ferroic specie; (2) If D_G^S is contained in $D_G^{H'}$, and the number of times appears without an asterisk, GFH' is a partial ferroic specie.

For example, electric polarization transforms as the polar vector representation D^V_G. For the point group G=O, from Table II, $D^V_G=\Gamma_4$. From the column under Γ_4 in Table I, one finds that OFC_1, OFC_2^{XY}, OFC_3, and OFC_4 are full ferroelectric species, and OFC_2^Z is a partial ferroelectric specie.

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