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Order parameter symmetries and free-energy expansions for purely ferroelastic transitions

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Purely ferroelastic transitions, i.e., transitions associated with a spontaneous deformation but no spontaneous polarization, appear from recent experimental investigations as a very common type of structural phase transitions. A theoretical analysis is presented for this class of transitions on the basis of Landau's theory of continuous phase transitions. The possible symmetries of their order parameter are systematically worked out both for the cell-preserving transitions and for those which modify the number of atoms in the crystal unit cell. Accordingly, we examine the transitions induced by the space-groups irreducible representations complying with the Landau and Lifshitz symmetry criteria. For each representation attention is given, in particular, to the construction of the finite group constituted by the set of distinct matrices of the representation, since this set (the image of the representation) determines the form of the Landau free energy and the number and characteristics of the low-symmetry phases. The images corresponding to the four-, six-, and eight-dimensional order parameters, which were not known previously, have been systematically determined for the 230 crystallographic space groups. We find 22 four-dimensional images associated with the "active" irreducible representations, ten six-dimensional, and five eight-dimensional ones. The corresponding Landau free energies have been expanded as a function of the order-parameter components, up to the lowest-degree terms which influence the stability of the low-symmetry phases just below a line of continuous transitions. It is pointed out that, in some cases, polynomials of degree as high as 12 must be considered. Whenever the order parameter and the spontaneous deformation have different symmetry properties, (improper ferroelastics), we have examined the additional contributions to the Landau free energy which represent the coupling between those two quantities. Their form depends on the particular space-group representations and not only on the images of these representations. We have worked out the lowest-degree coupling term for all the considered transitions. Its degree in the order parameter (the "faintness" index), which governs the qualitative temperature dependence of the macroscopic deformation and elastic constants is found equal to 2 in most cases, though values of 3 and 4 are also found possible. For each of the predicted types of ferroelastic transitions the space-symmetry change and unit-cell expansion have been determined. These crystallographic results are presented in table form and discussed. It is pointed out, in particular, that purely ferroelastic transitions constitute the major part of the ferroic phase transitions which are inferred to be possible in the framework of the Landau theory. Finally, the former theoretical results are compared to the available experimental data.

I. INTRODUCTION

The Landau theory of continuous phase transitions[1] provides a basis for deriving several important features of structural phase transitions, namely, the change in the crystal's space group, the dimension and symmetry properties of the transition's order parameter, and the form of the free-energy expansion. The theory does not account correctly, in general, for the behavior of physical quantities in the vicinity of the transition point since it has the same range of validity as the mean-field approximation in microscopic theories. However, its results concerning the prediction of the symmetry changes have been shown[2] to be independent of the preceding approximation. Besides, the characteristics of the order-parameter and of the free-energy expansion, defined by the theory, are known to keep an important role in the more advanced statistical theories of the critical behavior.

The symmetry criteria contained in Landau's theory limit to a few thousands the number of different symmetry changes which are likely to be encountered. These restrictions are only valid, in principle, for continuous transitions between strictly periodic structures, but they also hold for many transitions of first order.[3,4] Conversely, examples of first-order transitions not complying with them are known.[5] It is also expected that transitions leading to a modulated structure will generally not be submitted to them.[6] However, the precise extent of their applicability to the actually observed crystalline transitions cannot be fully estimated because, up to now, the symmetry changes determined from the Landau and Lifshitz symmetry criteria have not been extensively worked out, and accordingly, no systematic comparison could be made to the experimental data. Group-theoretical work based on these criteria have either been restricted to transitions preserving the translations of the crystal, or directed towards the understanding of the symmetry changes occurring in particular structural families.[7,8]

In two previous papers,[9,10] referred to hereafter as TTI and TTII, we have started investigating the order-parameter symmetries, space-group changes, and free-energy expansions relative to all the continuous transitions which are likely to arise from any of the 230 crystallographic space groups.

These studies dealt with the structural transitions which modify the crystal class and, possibly, its primitive translations, but keep unchanged the crystal system. In TTI the case of purely ferroelectric transitions was examined, while TTII was devoted to the secondary- and higher-order ferroic transitions, i.e., to the transitions involving the onset of a spontaneous polar tensor or rank higher than two. In both works the theoretical results were used to compare the predictions of Landau's theory to the available experimental data for the considered types of transitions.

In the present paper, we extend this study to the case of purely ferroelastic transitions. These transitions are of a special interest because, though only recently the subject of a systematic experimental investigation, they already appear as a very commonly encountered type of structural transition. We will show in this work that they also constitute a major part of the transitions which are theoretically predicted to be possible in the framework of Landau's theory.

Ferroelastic transitions are those structural phase transitions which give rise to a spontaneous strain. They have been recognized by Aizu[11] in 1969 as a group of transitions sharing common properties, and constituting the mechanical analogs of ferroelectric phase transitions. In particular, the low-symmetry (ferroelastic) phase is characterized by a stress-strain hysteresis loop which discloses the occurrence of several strain-differing stable states (the ferroelastic domains), and also the possibility of switching the crystal from one stable state to another by applying an external stress.

Ferroelasticity sometimes occurs in conjunction with ferroelectricity such as in several well-known ferroelectrics[12] (KDP, Rochelle-salt, barium titanate). However, an increasing number of substances have been found to display a purely ferroelastic (i.e., not simultaneously ferroelectric) transition. Prominent examples are lanthanum pentaphosphate[13] LaP_5O_{14}, potassium trihydrogen selenite[14] $KH_3(SeO_3)_2$, mercury chloride[15] Hg_2Cl_2, lead phosphate[16] $Pb_3(PO_4)_2$, antimony iodide oxide[17] Sb_5O_7I, bismuth vanadate[18] $BiVO_4$, and many compounds with the perovskite structure ($SrTiO_3$, $LaAlO_3$, $CsPbCl_3$). A few organic materials, namely, the polyphenyls[19] and squaric acid,[20] also belong to this group as well as several metallic alloys such as V_3Si (Ref. 21) and $CuAuZn_2$.[22] Moreover, two extensively studied classes of crystalline transformations, i.e., the thermoelastic martensitic transformations[23] and the cooperative Jahn-Teller transitions,[24] have been recognized[25] as closely related to purely ferroelastic transitions.

A theoretical analysis of purely ferroelastic transitions is described in Secs. II–IV. In Sec. II we briefly recall the crystallographic and physical characteristics which define these transitions, and we outline the method used to apply to them the Landau theory. The working out of Landau's symmetry criteria is based on the space-group representations instead of the simpler point-group ones, in order to account for the transitions which involve a change in the translational symmetry. Such a procedure is fully justified by the fact that a large number of the currently known ferroelastics actually display a modification of the translational symmetry. Investigations of the purely ferroelastic transitions which preserve the crystal's translations had previously been performed by Boccara,[26] Aizu,[27] and in a more complete way by Janovec *et al.*[28] Section III is devoted to the study of the free-energy expansions relative to the considered transitions. A reduction of the number of cases to be handled is achieved through the use of the images[29] of the representations. Particular attention is given to the four-, six-, and eight-dimensional irreducible representations for which the images are determined for the first time. The lowest-degree terms are listed for all the encountered types of expansions, including the terms representing the coupling between the order parameter and the ferroelastic strain. The minima of the order-parameter expansions are algebraically discussed in order to derive the various low-symmetry phases which are likely to be stable below the transition point. Section IV contains in table form the results of the systematic determination of the space-symmetry changes accompanying all possible ferroelastic transitions as well as their discussion. In Sec. IV, we also compare the results of the theoretical investigation to the available experimental data.

II. THEORETICAL PROCEDURE

In the Landau theory the symmetry change which takes place at a continuous transition is related to the symmetry properties of a certain active[30] physically irreducible[30] representation (IR) of the high-symmetry (HS) space group. This IR is spanned by the components of the transition's order parameter (OP). The symmetry change will be a ferroelastic one if the thermal-expansion tensor of the low-symmetry (LS) phase has more independent components than that of the HS phase. This condition arises[31] from the fact that the spontaneous strain is represented by a symmetric second-rank tensor which, moreover, vanishes by symmetry in the HS phase (it is therefore necessarily traceless). In addition to the trivial group-subgroup relationship between phases, which is implicitly assumed, the former criterion requires,[31–33] at the crystallographic level, that the two symmetry-related point groups belong to different crystal systems, provided that the hexagonal and trigonal systems are considered as a single system.

Pure ferroelasticity is defined by the additional condition that the same components of a vector (polarization) are compatible with the crystal classes of the two phases (this includes, in particular, transitions between polar classes). The macroscopic features of the ferroelastic phase, such as the number of orientational domains, or the form of the spontaneous-strain tensor are determined by the nature and orientation of the set of point-symmetry elements of the HS phase which are retained in the LS one.[28] Physically distinct situations will be associated to different ferroelastic "species".[11] There are 64 species associated with the purely ferroelastic transitions (PFT) considered in this work. For some of the species, several domain orientations are characterized by an identical spontaneous-strain tensor and they can only be distinguished at macroscopic level, by spontaneous components of higher-rank tensors. These species are not "full" ferroelastic ones in the sense of Aizu.[11] We have, nevertheless, included them among the investigated PFT.

We have listed in Table I the 64 former species and their respective spontaneous tensorial components. Strain components were previously worked out by Aizu,[34] while the full set of spontaneous components can be found in the work of Janovec *et al.*[28]

The latter authors have pointed out that, from a group-theoretical point of view, the spontaneous components relative to a given species can belong either to one, or to several IR of the HS point group. The decomposition of the relevant tensorial components into irreducible parts with respect to the HS class has been reproduced in Table I as it provides an essential indication in determining the coupling scheme between these components and the order parameter of the transition (see Sec. III).

Table I shows that the 64 considered species derive from 21 HS crystal classes. We can restrict our analysis to the 188 space groups belonging to these classes as only their active IR are likely to give rise to a PFT. The procedure of working out systematically all the possible continuous PFT is then (i) to select the active IR's of each space group G_0, (ii) to determine the stable LS phases, compatible with a given IR, (iii) to select the LS phases whose point-symmetry forms, with the point symmetry of G_0, a purely ferroelastic species appearing in Table I, and (iv) to identify the space group of each of the former LS phases.

The selection of the active IR's of a space group G_0 has been described by Lyubarskii[30] and recalled in TTI. It is effected in three steps. First are retained the IR's, denoted $\Gamma_n(k^*)$, whose star k^* corresponds either to the center ($\vec{k}=0$) of the Brillouin zone (BZ) relative to G_0, or to one of a few definite $\vec{k}$ vectors of the BZ boundary. These prominent $\vec{k}$ vectors were listed in TTII for the BZ of the cubic system and in TTI for the remaining systems. This preliminary filtering relies on the rejection of the IR's whose antisymmetrized square $\{\Gamma_n(k^*)^2\}$ possesses a representation in common with the vector representation of G_0 (Lifshitz criterion).[30] The former criterion is then applied a second time, at a more detailed level, to the small representations τ_n relative to each acceptable $\vec{k}$ vector, thus producing a further selection. The resulting IR's complying with the Lifshitz condition were indicated in TTI and TTII.

Finally, among the preceding IR's are only kept the ones whose symmetrized third power $[\Gamma_n(k^*)^3]$ does not contain the totally symmetric IR of G_0 (Landau criterion).[30] The latter condition is not a selective one: it is trivially fulfilled by the IR's of all the space groups except by those relative to a few stars of the cubic and hexagonal BZ. However, in the latter cases, its practical application for $k^* \neq 0$ often requires a lengthy construction of the representation matrices, and it is therefore more conveniently achieved as the last step of the selection.

The space group G of the LS phase, determined by a given active IR, coincides with the set of symmetry operations belonging to G_0 which leave invariant a certain vector $\delta\rho$ in the abstract vector space of the considered IR. The components η_i^0 of this vector in the ϕ_i basis of the IR are the particular values of the OP components which correspond to the absolute minimum of the Landau free-energy expansion. For an m-dimensional IR ($m > 1$), depending on the relative algebraic values of the expansion's coefficients, the absolute minimum is likely to be associated with different vector directions in the m-dimensional representation space ϵ. As a consequence, several low-symmetry groups G are possible.

In TTI and TTII the groups G of interest were required to belong to the same crystal system as G_0. It

TABLE I. Purely ferroelastic species. Columns 1,2: set of point groups and orientation of the LS elements defining each species. Column 3: strain x_i, piezoelectric d_{ij} and elastic C_{ij} spontaneous components. τ_i irreducible representation of the HS point group inducing the point-symmetry change (several τ_i can be involved in certain species, this is indicated by the symbol +). Each τ_i is preceded by the set of tensorial components spanning it. The number of components between brackets (some of which can be zero) is the dimension of τ_i. Whenever the spontaneous-strain tensor has components not belonging to the former τ_i's, they are reproduced on the same line without being followed by a τ_i symbol. The Voigt contracted notation (Ref. 43) is used for macroscopic tensors and the τ_i are referred to the tables of Zak (Ref. 45).

$$[a]=[\sqrt{3}(x_2-x_1),x_1+x_2-2x_3]\ ;\ [b]=(0,x_1+x_2-2x_3)\ .$$

Species		Spontaneous components
$2/m$	$\bar{1}$	$x_6\{\tau_2\};x_4\{\tau_2\}$
$mm2$	2	$x_6\{\tau_3\}$
mmm	$2/m$	$x_6\{\tau_4\}$
mmm	$\bar{1}$	$x_4\{\tau_2\}+x_5\{\tau_3\}+x_6\{\tau_4\}$
4	2	$(x_1-x_2)\{\tau_2\};x_6\{\tau_2\}$
$4/m$	$2/m$	
$4/m$	$\bar{1}$	$[x_5,x_4]\{\tau_3+\tau_4\};(x_1-x_2);x_6$
422	2^x22	$(x_1-x_2)\{\tau_3\}$
$4mm$	m^xm2	
$\bar{4}2m$	2^x22	
$4/mmm$	m^xmm	
422	$2^{xy}22$	$x_6\{\tau_4\}$
$4mm$	$m^{xy}m2$	
$4/mmm$	$m^{xy}mm$	
$4/mmm$	2^x22	$(d_{14}-d_{25})\{\tau_6\}+(x_1-x_2)\{\tau_3\}$
$4/mmm$	$2^{xy}22$	$(d_{14}-d_{25})\{\tau_6\}+x_6\{\tau_4\}$
$4mm$	2	$(x_1-x_2)\{\tau_3\}+x_6\{\tau_4\}$
$4/mmm$	$2^z/m$	
$4/mmm$	$2^{xy}/m$	$[x_4,x_5=x_4]\{\tau_5\};x_6$
$4/mmm$	$2^x/m$	$[x_4,x_5=0]\{\tau_5\};(x_1-x_2)$
$4/mmm$	$\bar{1}$	$[x_4,x_5]\{\tau_5\};(x_1-x_2);x_6$
$\bar{3}$	$\bar{1}$	$[\frac{1}{2}(x_2-x_1),x_6]\{\tau_2+\tau_3\};[x_5,x_4]\{\tau_2+\tau_3\}$
$\bar{3}m$	$\bar{1}$	$[\frac{1}{2}(x_2-x_1),x_6]\{\tau_3\};[x_5,x_4]\{\tau_3\}$
$\bar{3}m$	$2/m$	$[\frac{1}{2}(x_2-x_1),0]\{\tau_3\};[x_5,0]\{\tau_3\}$
6	2	$[\frac{1}{2}(x_2-x_1),x_6]\{\tau_3+\tau_4\}$
$6/m$	$2/m$	
$6/m$	$\bar{1}$	$[x_5,x_4]\{\tau_{11}+\tau_{12}\};[\frac{1}{2}(x_2-x_1),x_6]$
622	222	$[\frac{1}{2}(x_2-x_1),0]\{\tau_6\}$
$6mm$	$mm2$	
$6/mmm$	mmm	
$6/mmm$	222	$[0,d_{36}]\{\tau_{12}\}+[\frac{1}{2}(x_2-x_1),0]$
$6mm$	2	$[\frac{1}{2}(x_2-x_1),x_6]\{\tau_6\}$
$6/mmm$	$2^z/m$	
$6/mmm$	$2^x/m$	$[x_5,0]\{\tau_5\}+[\frac{1}{2}(x_2-x_1),0]$
$6/mmm$	$\bar{1}$	$[x_5,x_4]\{\tau_5\}+[\frac{1}{2}(x_2-x_1),x_6]$
23	222	$[a]\{\tau_2+\tau_3\}$
$m3$	mmm	
$m3$	222	$[\sqrt{3}(d_{25}-d_{14}),(d_{15}+d_{24}-2d_{36})]\{\tau_6+\tau_7\};[a]$
$m3$	$2/m$	$[0,0,x_6]\{\tau_4\};[a]$
$m3$	$\bar{1}$	$[x_4,x_5,x_6]\{\tau_4\};[a]$
$m3$	$\bar{3}$	$[x_4,x_4,x_4]\{\tau_4\};[a]$

TABLE I. *(Continued)*

Species		Spontaneous components
$\bar{4}3m$	$\bar{4}2m$	$[b]\{\tau_3\}$
432	422	
$m3m$	$4/mmm$	
$m3m$	422	$[\sqrt{3}(d_{14}-d_{25}),0]\{\tau_8\};+[b]$
$m3m$	$\bar{4}2^{x}m$	$[0,(d_{14}+d_{25}-2d_{36})]\{\tau_8\};[b]$
$m3m$	$\bar{4}2^{xy}m$	$[0,0,d_{24}-d_{15}]\{\tau_9\};[b]$
$m3m$	$4/m$	$[0,0,C_{16}-C_{26}]\{\tau_4\};[b]$
$\bar{4}3m$	$\bar{4}$	$[0,0,d_{24}-d_{15}]\{\tau_5\};[b]$
$m3m$	$\bar{4}$	$[0,0,C_{16}-C_{26}]\{\tau_4\}$ $+[0,0,d_{14}-d_{25}]\{\tau_9\};[b]$
$\bar{4}3m$	222	$[a]\{\tau_3\}$
432	222^{x}	
$m3m$	mmm^{x}	
$m3m$	222^{x}	$[\sqrt{3}(d_{14}-d_{25}),0]\{\tau_8\}$ $+[a]\{\tau_3\}$
432	222^{xy}	$[0,0,x_6]\{\tau_5\};[b]$
$m3m$	mmm^{xy}	
$m3m$	222^{xy}	$[\sqrt{3}(d_{14}-d_{25}),0]\{\tau_8\}$ $+[0,0,x_6]\{\tau_5\};[b]$
$m3m$	$2^{z}/m$	$[a]\{\tau_3\}+[0,0,x_6]\{\tau_5\}$
$m3m$	$2^{xy}/m$	$[x_4,x_5,x_6]\{\tau_5\};[b]$
$m3m$	$\bar{1}$	$[x_4,x_5,x_6]\{\tau_5\}+[a]\{\tau_3\}$
432	32	$[x_4,x_4,x_4]\{\tau_5\}$
$m3m$	$\bar{3}m$	
$m3m$	$\bar{3}$	$[(C_{24}-C_{34})=e,(C_{35}-C_{15})=e,$ $(C_{16}-C_{26})=e]\{\tau_4\};$ $[x_4,x_4,x_4]$
$m3m$	32	$[(d_{35}-d_{26})=d,(d_{16}-d_{34})=d,$ $(d_{24}-d_{15})=d]\{\tau_9\};[x_4,x_4,x_4]$

was shown that a necessary condition is that the corresponding vectors $\delta\rho$ lie along certain prominent directions in ϵ. The possible occurrence of a LS phase of the considered type could then be checked directly among the invariance groups G of these directions. A free-energy expansion had, in principle, to be handled in the infrequent cases where a phase with the required symmetry was obtained.

In the study of ferroelastic transitions, which essentially involve a modification of the crystal system, the above simplification does not remain valid, and any vector of ϵ is likely to be associated to such a transition. Consequently, to determine the possible LS phases relative to a continuous PFT, one has to go through the standard procedure outlined by Lyubarskii[30] and locate first the various directions in ϵ which correspond to a minimum of the Landau free energy. The LS group G can then be specified for each such direction. The first step of the method therefore consists in the construction of the free-energy expansion and the algebraic discussion of its minima. For the reasons stated above, such a discussion was not performed in detail in TTI and TTII. It is undertaken in Sec. III for the expansions arising from all the active IR's.

III. FREE-ENERGY EXPANSIONS IN THE LANDAU THEORY

The Landau free energy (LFE) is a polynomial expansion whose terms are invariant functions under the symmetry operations of the HS space group. For a PFT, this expansion can be restricted to two sets of variables: the OP components (η_i) spanning the active IR which drives the transition, and the spontaneous-strain components (x_j) relative to the considered ferroelastic species (if the species is not a "full" one,[11] other higher-rank tensor components, indicated in Table I, should also be included).

When giving attention to the symmetry characteristics of the transition, one can neglect the macroscopic quantities which are coupled to the OP, but whose onset would preserve the crystal's higher symmetry (for instance the strain components already allowed by symmetry in the HS phase).

Likewise, we can ignore the macroscopic quantities whose onset would modify the symmetry of the crystal in a different way than the considered (x_j) components. The terms representing their coupling to the (η_i) are warranted to vanish by symmetry for equilibrium (η_i^0) values of the OP corresponding to the purely ferroelastic phase of interest.

Similarly to the case of ferroelectrics,[35] different situations can be distinguished on the basis of the relative symmetries of the OP and of the spontaneous strain. When the latter quantity belongs to the same IR as the OP, the corresponding PFT is labeled as "proper".[35] The star of the IR is necessarily $k^*=0$. As the physical nature of the OP is irrelevant to the symmetry aspects developed here, the OP can be chosen to coincide with the (x_j), and the LFE takes the form $F(x_j,C_l)$, where the C_l coefficients of the expansion are elastic constants of different orders.

If the sets (x_j) and (η_i) belong to different IR's, the considered PFT is an "improper" one.[35] This is always the case when the OP corresponds to $k^*\neq 0$, but it can also occur for $k^*=0$, if the OP is associated with tensorial components of rank higher than 2. For an improper PFT, the LFE can be split into three kinds of terms representing, respectively, the OP expansion, the strain expansion, and the mixed invariants relative to the coupling between those two quantities. We can write

$$F(\alpha,\eta_i,x_j,\beta_k,C_l,\delta_m) = F_1(\alpha,\eta_i,\beta_k)+F_2(x_j,C_l)+F_3(\eta_i,x_j,\delta_m) \ , \tag{1}$$

where $\alpha\approx(T-T_c)$ is the coefficient of the OP invariant of degree two, and β_k, C_l, δ_m are temperature-independent coefficients of the other terms constituting the expansion.

Finally, an intermediate situation, which has been noted by Janovec *et al.*,[28] arises when the OP coincides with one set of strain components (x_i) while another set (x_j), relative to the same ferroelastic species, belongs to a different nonidentical IR. The PFT will exhibit simultaneously a proper and an improper behavior. This occurs, for instance, in the case of the $P4/m \rightarrow P\bar{1}$ transition (Tables I and VII).

Let us examine the construction and properties of the different terms contributing to the expansion, in the most complex case of an improper PFT. The other cases can be easily deduced from it.

A. Construction of the Landau free energy

The OP expansion $F_1(\alpha,\eta_i,\beta_k)$ is a sum of independent homogeneous polynomials of various degrees, separately invariant by G_0. In addition to a single quadratic term, F_1 contains, in general, several fourth-degree ones. As we consider an active[30] IR, linear and third-degree invariants are necessarily absent from the expansion.

On the other hand, higher-degree invariants can, in general, be neglected in the vicinity of a continuous transition as they play no role in the stability of the LS phases just below the transition point. It can happen, however, that for certain multidimensional IR, a single quartic term exists which will necessarily possess spherical symmetry. More generally, an isotropy of the quartic terms can occur in a certain subspace of the representation space. In these cases the symmetries of the LS phases are determined by invariants of degree higher than four even near the transition.

In the expansion F_1 associated with a given IR, $\Gamma_n(k^*)$, the number of independent invariants of degree ν is unambiguously defined. It is equal to the number of times the trivial IR of G_0 is contained in the symmetrized νth power $[\Gamma_n(k^*)^\nu]$ of the IR. By contrast, the form of these invariants is partly arbitrary, as any linear combination of several of them will provide another invariant polynomial. More significantly, the expression of a given invariant depends on the choice of a frame of reference in the representation space ϵ. For all the expansions discussed here the following choice has been made:

(i) If the star of $\Gamma_n(k^*)$ has one arm, the basis coincides with the one defining the representation matrices in Kovalev's tables.[36] However, for two-dimensional real IR's, the basis provided by the tables is sometimes a complex one. Also, the considered IR can be the sum of two complex-conjugate IR's. In both cases, the basis has been converted into a real one by one of the sets of transformations

$$[\eta'=(1/\sqrt{2})(\eta+i\xi);\ \ \xi'=(1/\sqrt{2})(\eta-i\xi)]$$

or

$$[\eta'=\eta;\ \ \xi'=i\xi].$$

(ii) If the star of $\Gamma_n(k^*)$ has several arms, the basis of the small representation τ_n is constructed from Kovalev's tables as in the preceding case and a standard[30] basis of the entire IR is then generated from it (the various possible choices of this standard basis have no influence on the form of the expansion within a permutation on the OP components).

The working out of the independent invariants has been achieved by projecting the basis functions of $[\Gamma_n(k^*)^\nu]$ on the trivial representation of G_0. To perform this projection it is sufficient to know the set of *distinct* matrices of $\Gamma_n(k^*)$ associated with the elements of G_0.

For an active IR, the number of distinct matrices is always finite[37] though G_0 is of infinite order. As noted by Gufan *et al.*,[37] their set can be considered as the physically irreducible vector representation of a finite point group L, acting in the m-dimensional space ϵ. L is sometimes called[29] the image of $\Gamma_n(k^*)$.

The advantage of considering the images instead of the entire set of matrices constituting the IR, lies in the fact that several IR's correspond to the same image. Essential features of the transitions such as the form of the OP expansion, the number of LS phases, and their symmetry relationship, the number of domains, can be investigated in a considerable reduced number of cases corresponding to the distinct images.

The number of different images associated to the active IR's is limited by crystallographic restrictions.[37] The case of the images of the two- and three-dimensional IR's has been studied first by Gufan *et al.*[37] It has been shown that there are eight "active" images in two dimensions. Their set of matrices are, respectively, isomorphic to the two-dimensional point groups C_4, C_{4v}, C_6, C_{6v}, C_8, C_{8v}, C_{12}, and C_{12v} (Schoenflies notation). Likewise, three-dimensional active IR's give rise to three images only, which are isomorphic to the three-dimensional crystallographic point groups T_h, O, and O_h. Generally speaking, there will be as many distinct OP expansions of the corresponding dimensions. However, if we only retain the terms of lowest degrees which are just necessary to account for the continuous symmetry change, several distinct images will be associated with the same form of expansion. Thus, the same fourth-degree expansion corresponds to all the three-dimensional images.[37]

The construction of the expansions relative to the two- and three-dimensional images has been performed by several authors.[29,37] For higher dimensions, OP expansions have only been constructed in a few particular cases corresponding to certain families of compounds.[3,5,8,38] Besides, no information is available on the higher-dimensional images. We have determined these images and the lowest-degree terms of the corresponding OP expansions for the four-, six-, and eight-dimensional active IR. No higher dimension is involved when dealing with continuous transitions between periodic phases since no IR's with higher dimensions are found to comply with the Lifshitz criterion. For the sake of completeness, we have extended this part of the investigation to the 230 crystallographic space groups and not only to the 188 space groups relevant to the study of pure ferroelasticity.

Active IR's give rise to 22 four-dimensional, 10 six-dimensional, and 5 eight-dimensional images. Only two of these images are not related to the onset of pure ferroelasticity. Gufan *et al.*[37] have stated that one should find, at most, 24 four-dimensional and 6 six-dimensional images complying with the Lifschitz criterion but not necessarily with the Landau one. This statement, whose basis is not explained by the former authors, is obviously incorrect for six dimensions (we even find 7 six-dimensional images, not indicated here, which do not comply with the Landau criterion).

The four-dimensional images arise from IR's of the orthorhombic, tetragonal, hexagonal, and cubic systems. Their order (number of distinct matrices) range from 8 to 384. The occurrence of the highest orders might seem surprising since these exceed the maximum number of point-symmetry elements encountered in the crystallographic groups (48). Their origin lies in the occasional complexity of the matrices representing the primitive translations of the crystal at certain BZ points.

We have noted that each image is isomorphic to one of the 227 point groups which occur in four-dimensional crystallography. We were able to identify these point groups by using the tables of Mozrzymas,[39] in which the 227 former classes are explicitly described by the set of their generating matrices.

Six-dimensional images occur in the cubic system only, while eight-dimensional ones arise from active IR's of the cubic and hexagonal systems. Their orders are, respectively, in the ranges 48–1536 and 72–384. Similarly to the case of three and four dimensions (but not of two dimensions) the latter images are isomorphic to "crystallographic"[40] point groups since they are generated by integral[40] matrices. However, no tables of crystallographic point groups seem to be available for dimensions higher than 4, and a geometrical identification of the corresponding images is therefore meaningless at present.

The relationship between the various images is represented in Figs. 1 and 2. We have specified in these figures the three-dimensional crystallographic space groups G_0 whose IR give rise to each image as well as the type of OP expansion associated with it. The expansions have been listed in Tables II and III. As shown by the former tables and figures, the truncated expansions coincide for several images though the infinite expansions should all be different. As stressed above, the truncation has not always been limited to the fourth-degree terms. Tables II and III specify that the isotropy of the lowest-degree terms sometimes requires one to consider degrees as high as 12. Such a circumstance was already noted to occur for the two-dimensional expansions.[37]

Summing up our results with those already known for lower dimensions, it appears that active IR's of the 230 crystallographic space groups give rise to 49 images whose dimensions range from one to eight. The study of continuous transitions in the Landau theory is therefore reduced to the handling, at most, of 49 types of expansions.

To complete the construction of the LFE, we must determine the strain contributions $F_2(x_j,C_l)$ and the mixed invariant $F_3(\eta_i,x_j,\delta_m)$. The subsequent discussion stresses that these terms are not necessary to predict the number and symmetries of the LS phases which are entirely specified by the OP expansion. However their presence in the LFE are essential to the understanding of the onset of spontaneous-strain components and the occurrence of the elastic anomalies characteristic of the ferroelastic behavior.

Various authors[41,42] have emphasized that it is sufficient to expand the strain contribution $F_2(x_j,C_l)$ as

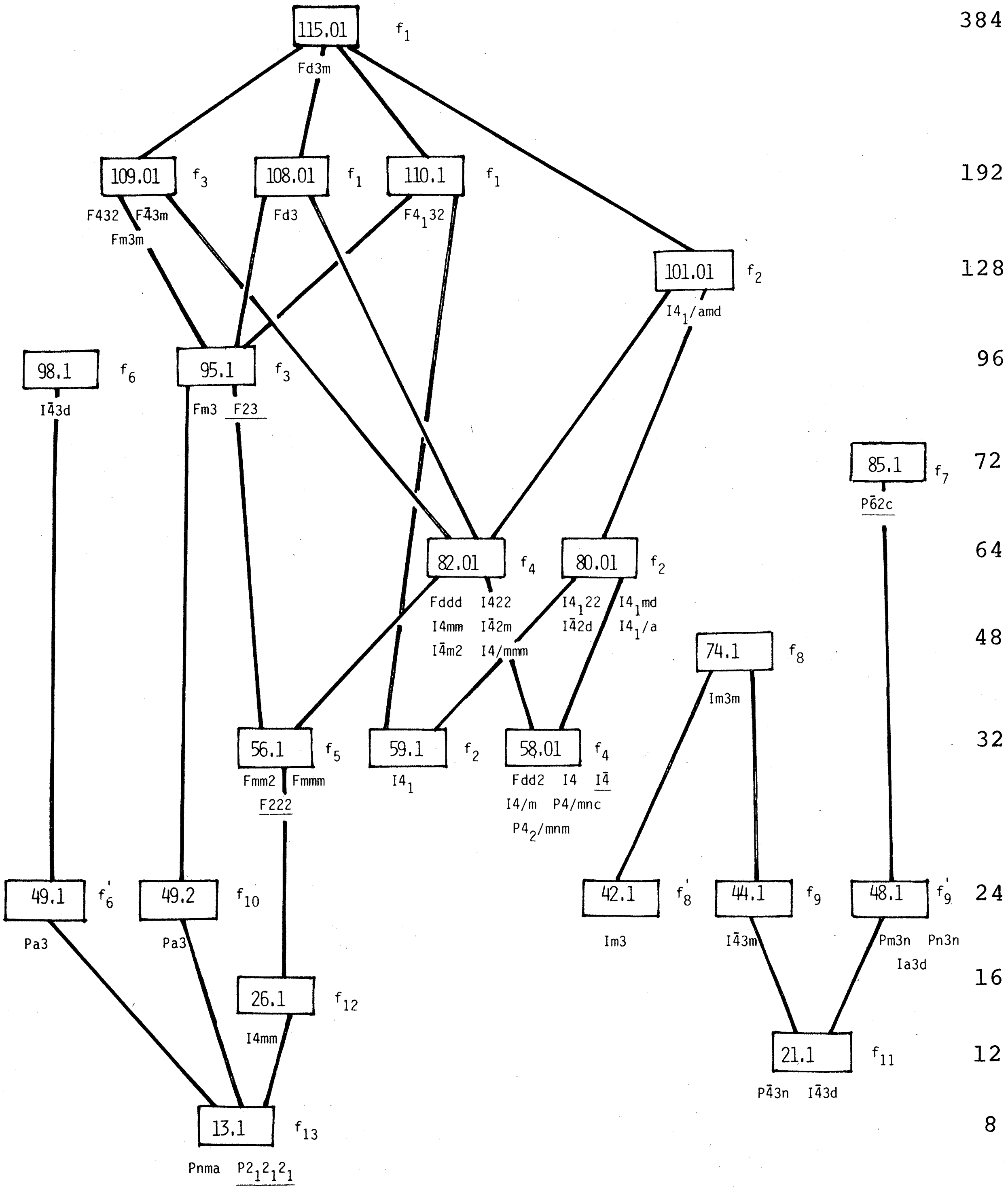

FIG. 1. Images of the four-dimensional physically irreducible active representations of the 230 crystallographic space groups. Each image is isomorphous to a four-dimensional crystallographic point gr up and is identified by the symbol for this group (e.g., 115.01) referred to the tables of Mozrzymas (Ref. 39). The orders of the various images are indicated on the vertical scale. Below each image are listed the three dimensional space groups whose IR's give rise to the image. These IR's are further specified (star, small representation) in Tables VI–IX. The symbols at the right of the images (e.g., f_1) represent the associated OP expansions whose expression is given in Table II. The connecting lines show the group-subgroup relationship between the images. Underlined space groups are not related to purely ferroelastic transitions.

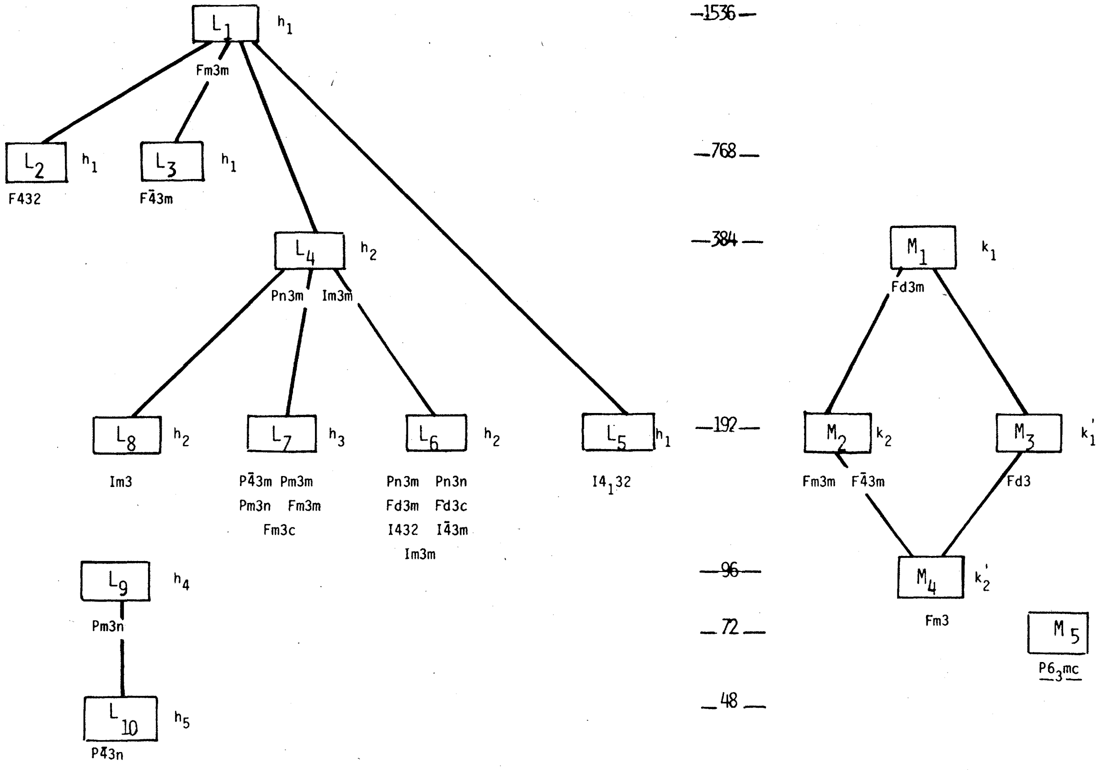

FIG. 2. Images of the six-dimensional (left) and eight-dimensional (right) physically irreducible active representations of the 230 space groups. The indications are the same as in Fig. 1 with the difference that the L_j and M_j symbols do not have any defined crystallographic meaning.

TABLE II. Four-dimensional order-parameter expansions. Column (a): labeling of the expansions; primed symbols possess the same fourth-degree terms as the corresponding unprimed ones but differ by the form of the higher-degree terms. Column (b): number of independent fourth-degree invariants. Column 3: form of the fourth-degree invariants

$$I_0=\sum_{1,4}\eta_i^4;\quad I_1=(\eta_1^2\eta_2^2+\eta_3^2\eta_4^2)\ ;\quad I_2=(\eta_1^2\eta_3^2+\eta_2^2\eta_4^2);\quad I_3=(\eta_1^2\eta_4^2+\eta_2^2\eta_3^2)\ ;\quad I_4=\eta_1\eta_2\eta_3\eta_4;\quad \eta_1=\rho_1\cos\phi_1\ ;$$

$$\zeta_1=\eta_2=\rho_1\sin\phi_1;\quad \eta_3=\rho_2\cos\phi_2\ ;\quad \eta_4=\rho_2\sin\phi_2=\zeta_2\ .$$

The terms of degree higher than four are not explicitly given, but the highest degree which must be taken to account in order to work out the stability of the LS phase is indicated (e.g., degree 12). Column (c): number of LS phases with distinct symmetries. Column (d): labeling of the different LS phases. Column (e): direction in the representation space associated to each LS phase. Directions of the type [1000] are symmetry elements of the image, while $[\eta\xi\eta'\xi']$ is not determined by symmetry.

(a)	(b)	Invariants	(c)	(d)	(e)
f_1	2	$\begin{cases} I_0 \\ (I_1+I_2+I_3) \end{cases}$	2	I II	[1000] [1111]
f_2	3	$\begin{cases} I_0;I_1 \\ (I_2+I_3) \end{cases}$	4	I II III IV	[1000] [1100] [1010] [1111]

TABLE II. *(Continued)*

(a)	(b)	Invariants	(c)	(d)	(e)
f_3	3	$\left\{\begin{array}{l} I_0;I_4 \\ (I_1+I_2+I_3) \end{array}\right.$	3	I II III	[1000] [1111] $[111\bar{1}]$
f_4	4	$\left\{\begin{array}{l} I_0;I_1 \\ I_2;I_3 \end{array}\right.$	5	I II III IV V	[1000] [1100] [1010] [1001] [1111]
f_5	5	$\left\{\begin{array}{l} I_0;I_1 \\ I_2;I_3;I_4 \end{array}\right.$	6	I II III IV V VI	[1000] [1100] [1010] [1001] [1111] $[111\bar{1}]$
f_6	1	$(\rho_1^2+\rho_2^2)^2$ +degree 6.	2	I II	$[\eta\zeta 00]$ $[\eta\zeta\zeta\eta]$
f_6'	1	$(\rho_1^2+\rho_2^2)^2$ +degree 6.	1	I	$[\eta\zeta\eta'\zeta']$
f_7	2	$(\rho_1^4+\rho_2^4);\rho_1^2\rho_2^2$ +degree 6.	2	I II	$[\eta\zeta 00]$ $[\eta\zeta\zeta\eta]$
f_8	3	$\left\{\begin{array}{l} (\rho_1^4+\rho_2^4);\rho_1^2\rho_2^2; \\ \rho_1^2\rho_2^2\cos 2(\phi_1-\phi_2) \\ +\text{degree } 12. \end{array}\right.$	6	I II III IV V VI	[1000] [1100] [1010] [0101] $[111\bar{1}]$ $[11\bar{1}1]$
f_8'	3	$\left\{\begin{array}{l} (\rho_1^4+\rho_2^4);\rho_1^2\rho_2^2; \\ \rho_1^2\rho_2^2\cos 2(\phi_1-\phi_2) \\ +\text{degree } 12. \end{array}\right.$	3	I II III	$[\eta\zeta 00]$ $[\eta\zeta\eta\zeta]$ $[\eta\zeta\zeta\bar{\eta}]$
f_9	4	$\left\{\begin{array}{l} f_8;\rho_1^2\rho_2^2\sin 2(\phi_1-\phi_2) \\ +\text{degree } 12. \end{array}\right.$	3	I II III	$[\eta\zeta 00]$ $[\eta\zeta\eta\bar{\zeta}]$ $[\eta\zeta\bar{\eta}\zeta]$
f_9'	4	$\left\{\begin{array}{l} f_8;\rho_1^2\rho_2^2\sin 2(\phi_1-\phi_2) \\ +\text{degree } 6. \end{array}\right.$	2	I II	$[\eta\zeta 00]$ $[\eta\zeta\zeta\eta]$
f_{10}	5	$\left\{\begin{array}{l} I_0;(I_1+I_2+I_3);I_4 \\ \{\eta_1\zeta_1[\eta_1\eta_2+\zeta_1\zeta_2+\eta_2^2-\zeta_2^2 \\ +\eta_1\zeta_2-\eta_2\zeta_1]-\eta_2\zeta_2[\eta_1\eta_2 \\ +\zeta_1\zeta_2-\eta_1^2+\zeta_1^2-\eta_1\zeta_2+\eta_2\zeta_1]\}; \\ \{\eta_1\zeta_1(\eta_1^2-\zeta_1^2)+\eta_2\zeta_2(\eta_2^2-\zeta_2^2) \\ +\eta_1\eta_2(\eta_1^2-\eta_2^2)-\zeta_1\zeta_2(\zeta_1^2-\zeta_2^2) \\ +\eta_1\zeta_2(\eta_1^2-\zeta_1^2)-\eta_2\zeta_1(\eta_2^2-\zeta_2^2)\} \end{array}\right.$	1	I	$[\eta\zeta\zeta\zeta]$
f_{11}	6	$\left\{\begin{array}{l} f_9;\rho_1\rho_2(\rho_1^2-\rho_2^2)\cos(\phi_1-\phi_2); \\ \rho_1\rho_2(\rho_1^2-\rho_2^2)\sin(\phi_1-\phi_2); \\ +\text{degree } 6. \end{array}\right.$	1	I	$[\eta\zeta\eta'\zeta']$
f_{12}	7	$\left\{\begin{array}{l} f_8;\ \sum_{1,2}\rho_i^4\cos 4\phi_i; \\ \sum_{1,2}\rho_i^4\sin 4\phi_i; \\ \rho_1^2\rho_2^2\cos 2(\phi_1+\phi_2); \\ \rho_1^2\rho_2^2\sin 2(\phi_1+\phi_2); \end{array}\right.$	2	I II	$[\eta\zeta 00]$ $[\eta\zeta\zeta\bar{\eta}]$
f_{13}	11	$\left\{\begin{array}{l} f_{12};[\rho_1^3\rho_2\cos(3\phi_1-\phi_2) \\ -\rho_2^3\rho_1\cos(3\phi_2-\phi_1)]; \\ [\rho_1^3\rho_2\sin(3\phi_1-\phi_2) \\ -\rho_2^3\rho_1\sin(3\phi_2-\phi_1)]; \\ \rho_1\rho_2(\rho_1^2-\rho_2^2)\cos(\phi_1+\phi_2); \\ \rho_1\rho_2(\rho_1^2-\rho_2^2)\sin(\phi_1+\phi_2); \end{array}\right.$	1	I	$[\eta\zeta\eta'\zeta']$

TABLE III. Sixth- and eight-dimensional order-parameter expansions. The meaning of the various columns is the same as in Table II except for columns (d) and (e) which are grouped together. $\sum_{\mathrm{mod}3}\rho_i^2\rho_{i+1}^2$ means $(\rho_1^2\rho_2^2+\rho_2^2\rho_3^2+\rho_3^2\rho_1^2)$. The expansion corresponding to the eight-dimensional image M_5 is not indicated as irrelevant to PFT.

a	b	Invariants	c	Stable directions
h_1	3	$\sum\rho_i^4;\ \sum\rho_i^4\cos(4\phi_i);\ \sum_{i<j}\rho_i^2\rho_j^2;$	5	$\underline{\mathrm{I}}[10\,00\,00]$ $\underline{\mathrm{II}}[11\,00\,00]$ $\underline{\mathrm{III}}[10\,10\,10]$ $\underline{\mathrm{IV}}[01\,01\,01]$ $\underline{\mathrm{V}}[11\,11\,11]$
h_2	4	$\left\{\begin{array}{l} h_1; \\ \sum_{i<j}\rho_i^2\rho_j^2\sin2\phi_i\sin2\phi_j; \end{array}\right.$	6	$\underline{\mathrm{I}}[10\,00\,00]$ $\underline{\mathrm{II}}[11\,00\,00]$ $\underline{\mathrm{III}}[10\,10\,10]$ $\underline{\mathrm{IV}}[01\,01\,01]$ $\underline{\mathrm{V}}[11\,11\,11]$ $\underline{\mathrm{VI}}[11\,1\bar{1}\,00]$
h_3	5	$\left\{\begin{array}{l} h_2; \\ \sum_{\mathrm{mod}3}\rho_i^2\rho_{i+1}^2(\sin2\phi_i-\sin2\phi_{i+1}) \end{array}\right.$	7	$\underline{\mathrm{I}}[10\,00\,00]$ $\underline{\mathrm{II}}[11\,00\,00]$ $\mathrm{III}[10\,10\,10]$ $\underline{\mathrm{IV}}[01\,01\,01]$ $\underline{\mathrm{V}}[11\,11\,11]$ $\underline{\mathrm{VI}}[11\,1\bar{1}\,00]$ $\underline{\mathrm{VII}}[1\bar{1}\,11\,00]$
h_4	6	$\left\{\begin{array}{l} h_2; \\ \sum_{i<j}\rho_i^2\rho_j^2\cos2\phi_i\cos2\phi_j \\ \sum_{\mathrm{mod}3}\rho_i^2\rho_{i+1}^2(\cos2\phi_i-\cos2\phi_{i+1}) \end{array}\right.$	6	$\mathrm{I}[10\,00\,00]$ $\mathrm{II}[11\,00\,00]$ $\underline{\mathrm{III}}[10\,10\,10]$ $\underline{\mathrm{IV}}[01\,01\,01]$ $\underline{\mathrm{V}}[11\,11\,11]$ $\underline{\mathrm{VI}}[\eta\zeta\,\zeta{-}\eta\,00]$
h_5	9	$\left\{\begin{array}{l} h_4;\ \sum\rho_i^4\sin4\phi_i; \\ \sum_{i<j}\rho_i^2\rho_j^2\sin2(\phi_i+\phi_j) \\ \sum_{\mathrm{mod}3}\rho_i^2\rho_{i+1}^2(\sin2\phi_i-\sin2\phi_{i+1}) \end{array}\right.$	3	$\underline{\mathrm{I}}[\eta\zeta\,00\,00]$ $\underline{\mathrm{II}}[\eta\zeta\,\zeta{-}\eta\,00]$ $\underline{\mathrm{III}}[\eta\zeta\,\eta\zeta\,\eta\zeta]$
k_1	5	$\sum\rho_i^4;\ \sum_{i<j}\rho_i^2\rho_j^2;\ \sum_{i<j}\rho_i^2\rho_j^2\cos2(\phi_i-\phi_j)$ $[\rho_1^2\rho_2^2\cos2(\phi_1+\phi_2-\pi/3)+\rho_1^2\rho_4^2\cos2(\phi_1+\phi_4)$ $+\rho_3^2\rho_4^2\cos2(\phi_3+\phi_4-\pi/3)+\rho_2^2\rho_3^2\cos2(\phi_2+\phi_3)$ $+\rho_1^2\rho_3^2\cos2(\phi_1+\phi_3+\pi/3)+\rho_2^2\rho_4^2\cos2(\phi_2+\phi_4+\pi/3)]$ $[\rho_1^2\rho_2^2\cos(\phi_1+\phi_2+\pi/3)\cos(\phi_1-\phi_2)$ $+\rho_3^2\rho_4^2\cos(\phi_3+\phi_4+\pi/3)\cos(\phi_3-\phi_4)$ $+\rho_1^2\rho_3^2\cos(\phi_1+\phi_3-\pi/3)\cos(\phi_1-\phi_3)$ $+\rho_2^2\rho_4^2\cos(\phi_2+\phi_4-\pi/3)\cos(\phi_2-\phi_4)$ $+\rho_1^2\rho_4^2\cos(\phi_1+\phi_4)\cos(\phi_1-\phi_4)$ $+\rho_2^2\rho_3^2\cos(\phi_2+\phi_3)\cos(\phi_2-\phi_3)]$ +degree 6.	5	$\mathrm{I}[10\,00\,00\,00]$ $\mathrm{II}[01\,00\,00\,00]$ $\mathrm{III}[01\,00\,00\,10]$ $\mathrm{IV}[10\,10\,10\,10]$ $\mathrm{V}[01\,01\,01\,01]$
k_1'	5	k_1 +degree 6.	3	$\mathrm{I}[\eta\zeta\,00\,00\,00]$ $\mathrm{II}[\eta\zeta\,00\,00\,\eta\zeta]$ $\mathrm{III}[\eta\zeta\,\eta\zeta\,\eta\zeta\,\eta\zeta]$
k_2	6	k_1 $+\rho_1\rho_2\rho_3\rho_4\left(\sum_{i\neq1}{}_{\mathrm{mod}4}\cos(\phi_1+\phi_i-\phi_{i+1}-\phi_{i+2})\right)$ +degree 6.	6	$\mathrm{I}[10\,00\,00\,00]$ $\mathrm{II}[01\,00\,00\,00]$ $\mathrm{III}[10\,00\,00\,10]$ $\mathrm{IV}[10\,10\,10\,10]$ $\mathrm{V}[01\,01\,01\,01]$
k_2'	6	k_2 +degree 6.	3	$\mathrm{I}[\eta\zeta\,00\,00\,00]$ $\mathrm{II}[\eta\zeta\,00\,00\,\eta\zeta]$ $\mathrm{III}[\eta\zeta\,\eta\zeta\,\eta\zeta\,\eta\zeta]$

a function of the quadratic terms only. F_2 will thus coincide with the standard expression[43] of the elastic energy of the crystal in the HS phase, limited to the terms depending on the spontaneous components x_j. It has also been established[41,42] that the lowest-degree invariant in F_3 is necessarily a linear function of the x_j components. Whenever these components belong to several distinct IR's, denoted t_m of the HS point-group, each t_m will give rise to an invariant term of the form

$$\delta\left[\sum_j x_j\psi_j(\eta_i)\right], \qquad (2)$$

where the x_j and ψ_j are homologous bases spanning t_m. The ψ_j are homogeneous polynomials of degree p, obtained by projecting $[\Gamma_n(k^*)^p]$ upon t_m. Unlike the search of invariant polynomials, the generation of the ψ_j functions cannot be achieved by sole con-

TABLE IV. Coupling scheme between the order parameter and the spontaneous strain [full (Ref. 11) ferroelastic species] or the other spontaneous macroscopic quantities [partial (Ref. 11) species]. Column one: labeling of the set of ψ_j polynomials transforming according to the point-group representations. A, E, and T symbols correspond to one-, two-, and three-dimensional point-group representations. The first index is the number of components of the order parameter. Column 2: form of the ψ_j functions. The notations are the same as in Tables II and III. The indices of the summation are only specified once in each set. Column 4: faintness index relative to the spontaneous-macroscopic quantity defining the ferroelastic species [full (Ref. 11) or partial (Ref. 11)].

Labeling	Macroscopic spontaneous tensor components	Faintness index
$A_{2.1}$	$\eta\zeta$ or $(\eta^2-\zeta^2)$	2
$A_{2.2}$	$\eta\zeta$ and $(\eta^2-\zeta^2)$	2
$A_{3.1}$	$\eta_1\eta_2\eta_3$	3
$A_{4.1}$	$\eta_1^2+\eta_2^2-\eta_3^2-\eta_4^2$ [a]	2
$A_{4.2}$	$\eta_1\eta_2\eta_3\eta_4$	4
$A_{4.3}$	$\rho_1\rho_2\cos(\phi_1+\phi_2)$	2
$A_{6.1}$	$\sum_{1,3}\rho_i^2\cos 2\phi_i$	2
$A_{6.2}$	$\sum_{1,3}\rho_i^2\sin 2\phi_i$	2
$A_{6.3}$	$\rho_1\rho_2\rho_3 x$ $[\cos\phi_1\cos(\phi_2-\phi_3)+\sin\phi_1\sin(\phi_2+\phi_3)]$	3
$A_{8.1}$	$\rho_1\rho_2\rho_3\rho_4 x$ $\left\{\sum_{i\neq 1,\,\mathrm{mod}3}\cos(\phi_1+\phi_i-\phi_{i+1}-\phi_{i+2})\right\}$	4
$E_{2.1}$	$\{\eta^2-\zeta^2;2\eta\zeta\}$ [b]	2
$E_{2.2}$	$\{\eta^4+\zeta^4-6\eta^2\zeta^2;4\eta\zeta(\eta^2-\zeta^2)\}$ [b]	2
$E_{3.1}$	$\{2\eta_1^2-\eta_2^2-\eta_3^2;\sqrt{3}(\eta_2^2-\eta_3^2)\}$ [b]	2
$E_{4.1}$	$\left\{\sum_{1,2}(-1)^i\rho_i^4\cos 4\phi_i;\ \sum(-1)^i\rho_i^4\sin 4\phi_i\right\}$	4
$E_{4.2}$	$\left\{\sum_{1,2}\rho_i^4\cos 4\phi_i;\ \sum\rho_i^4\sin 4\phi_i\right\}$	4
$E_{4.3}$	$\left\{\begin{array}{l}\rho_1^2\cos 2\phi_1-\rho_2^2\cos 2\phi_2\\ \rho_1^2\sin 2\phi_1-\rho_2^2\sin 2\phi_2\end{array}\right.$	2
$E_{4.4}$	$\{\eta_4^2-\eta_3^2;\eta_1^2-\eta_2^2\}$ [a]	2
$E_{4.5}$	$\{\eta_3\eta_4;\eta_1\eta_2\}$ [a]	2
$E_{4.6}$	$\{\rho_1\rho_2\cos(\phi_1+\phi_2);\rho_1\rho_2\sin(\phi_1+\phi_2)\}$	2
$E_{6.1}$	$\{2\rho_1^2-\rho_2^2-\rho_3^2;\sqrt{3}(\rho_2^2-\rho_3^2)\}$ [a,b]	2
$E_{6.2}$	$\left\{\begin{array}{l}2\rho_1^2\sin 2\phi_1-\rho_2^2\sin 2\phi_2-\rho_3^2\sin 2\phi_3\\ \sqrt{3}(\rho_2^2\sin 2\phi_2-\rho_3^2\sin 2\phi_3)\end{array}\right.$ [a,b]	2
$E_{6.3}$	$\left\{\begin{array}{l}2\rho_1^2\cos 2\phi_1-\rho_2^2\cos 2\phi_2-\rho_3^2\cos 2\phi_3.\\ \sqrt{3}(\rho_2^2\cos 2\phi_2-\rho_3^2\cos 2\phi_3).\end{array}\right.$ [a]	2
$E_{8.1}$	$\left\{\sum_{1,4}\rho_i^2\cos 2\phi_i;\ \sum\rho_i^2\sin 2\phi_i\right\}$ [b]	2
$T_{3.1}$	$[\eta_2\eta_3;\eta_1\eta_3;\eta_1\eta_2]$ [a]	2
$T_{4.1}$	$\left\{\begin{array}{l}\eta_1^2+\eta_2^2-\eta_3^2-\eta_4^2.\\ \eta_1^2+\eta_3^2-\eta_2^2-\eta_4^2.\\ \eta_1^2+\eta_4^2-\eta_2^2-\eta_3^2.\end{array}\right.$ [a]	2
$T_{4.2}$	$\left\{\begin{array}{l}\rho_1^4\cos 4\phi_1-\rho_2^4\cos 4\phi_2.\\ \rho_1\rho_2[\rho_1^2\cos(3\phi_1+\phi_2)+\rho_2^2\cos(3\phi_2+\phi_1)].\\ \rho_1\rho_2[\rho_1^2\cos(3\phi_1+\phi_2)-\rho_2^2\cos(3\phi_2+\phi_1)].\end{array}\right.$	4
$T_{6.1}$	$\rho_1^2\cos 2\phi_1;\rho_2^2\cos 2\phi_2;\rho_3^2\cos 2\phi_3.$	2
$T_{6.2}$	$\left\{\begin{array}{l}\rho_1\rho_2\rho_3[\cos\phi_1\sin(\phi_2-\phi_3)-\sin\phi_1\cos(\phi_2+\phi_3)].\\ \rho_1\rho_2\rho_3[\cos\phi_2\sin(\phi_3-\phi_1)-\sin\phi_2\cos(\phi_3+\phi_1)].\\ \rho_1\rho_2\rho_3[\cos\phi_3\sin(\phi_1-\phi_2)-\sin\phi_3\cos(\phi_1+\phi_2)].\end{array}\right.$ [a]	3

TABLE IV. *(Continued)*

Labeling	Macroscopic spontaneous tensor components	Faintness index
$T_{8.1}$	$\left\{\begin{array}{l}\rho_1^2+\rho_2^2-\rho_3^2-\rho_4^2.\,^{\text{a}}\\ \rho_1^2+\rho_3^2-\rho_4^2-\rho_2^2.\\ \rho_1^2+\rho_4^2-\rho_2^2-\rho_3^2.\end{array}\right.$	2
$T_{8.2}$	$\left\{\begin{array}{l}\sum_{1,4}(-1)^i\rho_i^2(\cos2\phi_i-\sqrt{3}\sin2\phi_i).\\ \sum_{1,2}[\rho_{i+2}^2(\cos2\phi_{i+2}+\sqrt{3}\sin2\phi_{i+2})\\ \quad-\rho_i^2(\cos2\phi_i+\sqrt{3}\sin2\phi_i)].\\ 2(\rho_1^2\cos2\phi_1+\rho_4^2\cos2\phi_4-\rho_3^2\cos2\phi_3\\ \quad-\rho_2^2\cos2\phi_2).\end{array}\right.$	2

[a] within a permutation of the η_i or the ρ_i.

[b] within a permutation of the components in the bracket.

sideration of the images. For instance, in the $Pm3m$ space group, ψ_j functions of degree 3 are found at the M point[10] of the BZ while none is found at the X point,[10] though both IR's are associated with the same image denoted L_7 (Fig. 2).

In the vicinity of the transition point it is sufficient to consider the sets of ψ_j functions having the smallest degree $p=n_F$. This degree has been called[42] the faintness index relative to the ferroic properties. High values of n_F will, in principle, be associated with small anomalies affecting the mechanical properties of the crystal. Besides, n_F values of 2, 3, and $\geqslant 4$, have been shown[42] to correspond to three qualitatively different types of elastic anomalies at the transition. In the case of ferroelastic species involving several t_m, more than one faintness index can be necessary to describe the behavior of the spontaneous-strain components.

The ψ_j functions have been systematically worked out and listed in Table IV together with the corresponding faintness indices. Their expression is given in the same basis as the OP expansion. We have, respectively, denoted by A, E, and T the sets of ψ_j functions spanning an IR of the point-symmetry group having one, two, and three dimensions. As shown by the table, in most cases the faintness index is equal to 2, but values of 3 and 4 are also found possible. This situation can be compared to the transitions studied in TTI and TTII where faintness indices of three and four were frequently encountered.

B. Determination of the low-symmetry phases

We place ourselves in the strict framework of Landau's theory and consider the LS phases which are related to G_0 through a line of continuous transitions. Each phase is specified by the following conditions:

(i) It is associated with a set of component values $\eta_i^0(\alpha,\beta_k,C_l,\delta_m)$ and $x_j^0(\alpha,\beta_k,C_l,\delta_m)$ for which the LFE is an absolute minimum for a whole range of vanishingly small values of α, η_i^0, and x_j^0 (including the transition point).

(ii) For the whole range of these values the function $\delta\rho=\sum\eta_i^0\phi_i$, defined in Sec. II, has a definite invariance group G, subgroup of G_0, which coincides with the space group of the considered LS phase.

(iii) The same symmetry G corresponds to the coordinates (η_i^0,x_j^0) of the minimum of the LFE for a continuous range of values of each of the expansion coefficients (β_k,C_l,δ_m).

We therefore exclude the LS phases which can be reached from G_0 either by a discontinuous transition, or by a continuous one only occurring for particular values of the preceding coefficients.

As shown in the Appendix, the possible occurrence of a given symmetry change $G_0\rightarrow G$ along a line of continuous transitions, *regardless* of the corresponding (β_k,C_l,δ_m) values, does not depend on the strain contributions F_2 and F_3. An analysis can thus be limited to the OP expansion $F_1(\alpha,\eta_i,\beta_k)$.

A standard algebraic discussion has been performed for the various OP expansions contained in Tables II and III. The location of the absolute minima of F_1 consists of expressing the cancellation of its first derivatives, the positiveness of the matrix or the second derivatives, and in comparing the different minima which can simultaneously occur for given (β_k) coefficients.

The η_i^0 values obtained for the various expansions are indicated in Tables II and III for OP dimensions greater than 3. We have also recalled in Table V the results[37] for continuous transitions in the case of one- to three-dimensional OP. Similar to the cases of lower-dimension OP,[37] we can classify the LS phases in two catergories by putting $\eta_i^0=\rho^0\gamma_i^0$ $[\rho^0=\sum_i(\eta_i^0)^2]$. The first category corresponds to γ_i^0 values defining prominent directions in ϵ, lying along symmetry axes belonging to the image L. The γ_i^0 be-

TABLE V. Images and LS phases for the one-, two-, and three-dimensional active physically irreducible representations (C_i), (C_n, C_{nv}), (O, O_h, T_h) are Schoenflies notations for the one-, two-, and three-dimensional point groups. The order-parameter expansions relative to the images can be found in Refs. 28 and 37.

Images	Dimension	Number of LS phases	Labeling	Direction of ϵ
Ci	1	1	I	[1]
C_4, C_6 C_8, C_{12}	2	1	I	$[\eta, \zeta]$
C_{4v}, C_{12v}	2	2	I II	[10] [11]
C_{6v}	2	2	I II	[10] [01]
C_{8v}	2	2	I II	[10] $[\cos\frac{1}{8}\pi, \sin\frac{1}{8}\pi]$
T_h, O O_h	3	2	I II	[100] [111]

ing symmetry defined, the temperature dependence of the η_i^0 results exclusively from that of ρ^0. The second category corresponds to directions in ϵ which are not symmetry ones and which will generally vary with temperature as well as ρ^0. Both situations are found in the results of Tables II and III.

In four dimensions (Table II) expansions $f_1 - f_5$, which arise from real IR, have minima of the first type only. For the expansions $f_6 - f_{13}$, which are related to physically irreducible representations (i.e., sums of complex conjugates IR), only f_8 has minima of the first type while the other expansions provide two different situations. f_6', f_{11}, and f_{13} are associated with images determining no prominent symmetry directions in ϵ. Consequently the possible LS phases will all have the same symmetry.[37] By contrast, one or several LS phases are found for the remaining expansions corresponding to vectors lying in planes of symmetry of ϵ, but whose precise directions in these planes is not fixed by symmetry. Between one and six LS phases with distinct symmetries are found to be possible for all the four-dimensional images.

In six and eight dimensions (Table III) expansions $h_1 - h_3$ and k_1, k_2 determine minima of the first type, while h_4, h_5 and k_1', k_2' possess minima which correspond to planes of symmetry, similar to the case discussed above. The number of LS phases with distinct symmetries which can be reached through a line of continuous transitions is found, respectively, in the range 3–7 and 3–5.

IV. RESULTS AND DISCUSSION

The crystallographic and physical characteristics of the PFT which are predicted to be possible along a line of continuous transitions are summarized in Tables VI–IX, ordered according to the crystal system of the HS phase.

Table VI corresponds to a HS phase belonging to the monoclinic or orthorhombic system. Tables VII, VIII, and IX, respectively, contain the results relative to the tetragonal, trigonal-hexagonal, and cubic systems. The use of these tables allows the determination of the following characteristics of each possible PFT: (i) Space-symmetry change and unit-cell multiplication. (ii) Identification, dimension, and symmetry properties of the transition's order parameter. (iii) Form of the Landau free-energy, which includes the OP expansion as well as the additional terms relative to the spontaneous-strain components and to their coupling with the OP.

A. Organization and use of the tables

Let us describe the content of each of the eight columns constituting Tables VI–IX which summarize the results of the investigation. Some of their indications refer to Tables I–V as well as to available standard tables.[43–45]

Column 1 lists the HS space groups. But for a few

TABLE VI. Ferroelastic transitions with monoclinic or orthorhombic high-symmetry phase. The detailed meaning of the columns is explained in the text (Sec. IV). For the Γ point the indications are only reproduced for the first HS space group of each class. Primed coupling polynomials (e.g., $A'_{4.1}$ or $A''_{4.1}$) differ from unprimed ones by a permutation of the OP components.

HS group	BZ point	Low-symmetry phases	OP dim	(a)	(b)	(c)	(d)
$P2/m$	Γ	$P\bar{1}(\tau_2)$	1	C_i	I	1	proper
$P2_1/m$							
$P2/b$							
$B2/m$	Γ	$P\bar{1}$					
	F	$\underline{P}\bar{1}(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	F''	$\underline{P}\bar{1}(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
$P2_1/b$	Γ	$P\bar{1}$					
	C	$P\bar{1}(\tau_1+\tau_2,\tau_3+\tau_4)$	2	C_4	I	2	$A_{2.2}$
	D	$P\bar{1}(\tau_1+\tau_2,\tau_3+\tau_4)$	2	C_4	I	2	$A_{2.2}$
$B2/b$	Γ	$P\bar{1}$					
	F	$P\bar{1}(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	F''	$P\bar{1}(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
$Pmm2$	Γ	$P2(\tau_3)$	1	Ci	I	1	proper
$Pmc2$		$P2_1$					
$Pcc2$		$P2$					
$Pma2$		$P2$					
$Pca2_1$		$P2_1$					
$Pnc2$		$P2$					
$Pmn2_1$		$P2_1$					
$Pba2$		$P2$					
$Pna2_1$		$P2_1$					
$Pnn2$		$P2$					
$Cmm2$	Γ	$P2$		. . .			
	R	$B2(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	S	$P2(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
$Cmc2_1$	Γ	$P2_1$		. . .			
	S	$P2_1(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
$Ccc2$	Γ	$P2$		. . .			
	R	$B2(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	S	$P2(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
$Amm2$	Γ	$B2$		. . .			
$Abm2$		$B2$		. . .			
$Ama2$		$B2$		. . .			
$Aba2$		$B2$		. . .			
$Fmm2$	Γ	$B2$					
	R	$B2(\tau_1)$	4	56.1	IV	4	$A_{4.1}$
$Fdd2$	Γ	$B2$					
	R	$B2$	4	58.01	IV	4	$A_{4.1}$
		$B2(\tau_1)$			V	8	$A_{4.2}$
$Imm2$							
$Iba2$	Γ	$B2$					
$Ima2$	S	$B2(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
$Pmmm$	Γ	$P2/m(\tau_2)P2/m(\tau_3)$ $P2/m(\tau_4)$	1	C_i	I	1	proper
$Pnnn$		$P2/b,P2/b,P2/b$					
$Pccm$		$P2/b,P2/b,P2/m$					
$Pban$		$P2/b,P2/b,P2/b$					
$Pmma$		$P2_1/m,P2/m,P2/b$					
$Pnna$	Γ	$P2/b,P2_1/b,P2/b$		. . .			
	T	$[P2/b,B2/b](\tau_1,\tau_2)$	2	C_{4v}	I,II	2,2	$A_{2.1},A_{2.1}$
$Pmna$	Γ	$P2/m,P2/b,P2_1/b$		. . .			
	R	$[B2/m,B2/b](\tau_1,\tau_2)$	2	C_{4v}	I,II	2,2	$A_{2.1},A_{2.1}$
	U	$[B2/m,P2/b](\tau_1,\tau_2)$	2	C_{4v}	I,II	2,2	$A_{2.1},A_{2.1}$

TABLE VI. *(Continued)*

HS group	BZ point	Low-symmetry phases	OP dim	(a)	(b)	(c)	(d)
Pcca	Γ	$P2_1/b,P2/b,P2/b$		. . .			
Pbam	Γ	$P2_1/b,P2_1/b,P2/m$		. . .			
	R	$B2/m(\tau_2+\tau_6,\tau_1+\tau_5,$ $\tau_3+\tau_7,\tau_4+\tau_8)$	2	C_4	I	2	$A_{2.2}$
	S	$P2/m(\tau_1+\tau_5,\tau_4+\tau_3)$	2	C_4	I	2	$A_{2.2}$
		$P2/b(\tau_2+\tau_6,\tau_3+\tau_7)$	2	C_4	I	2	$A_{2.2}$
Pccn	Γ	$P2_1/b,P2_1/b,P2/b$		. . .			
	R	$B2/b\begin{cases}(\tau_1+\tau_5,\tau_2+\tau_6)\\(\tau_3+\tau_7,\tau_4+\tau_8)\end{cases}$	2	C_4	I		$A_{2.2}$
	S	$P2/b(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
Pbcm	Γ	$P2/b,P2_1/b,P2_1/m$		. . .			
Pnnm	Γ	$P2_1/b,P2_1/b,P2/m$		. . .			
	R	$B2/m(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	U	$[P2_1/b,B2/m]\ (\tau_1,\tau_2)$	2	C_{4v}	I,II	2,2	$A_{2.1},A_{2.1}$
	T	$[P2_1/b,B2/m]\ (\tau_1,\tau_2)$	2	C_{4v}	I,II	2,2	$A_{2.1},A_{2.1}$
	S	$P2/m(\tau_1+\tau_5,\tau_4+\tau_8)$ }	2	C_4	I	2	$A_{2.2}$
		$P2/b(\tau_2+\tau_6,\tau_3+\tau_7)$ }					
Pmmn	Γ	$P2_1/m,P2_1/m,P2/b$		. . .			
	R	$B2/m(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	S	$[P2/b](\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
Pbcn	Γ	$P2_1/b,P2/b,P2_1/b$		. . .			
	S	$[B2/b,P2_1/b](\tau_1,\tau_2)$	2	C_{4v}	I,II	2,2	$A_{2.1},A_{2.1}$
Pbca	Γ	$P2_1/b,P2_1/b,P2_1/b$		. . .			
	R	$P\bar{1}(\tau_1+\bar{\tau}_1,\tau_2+\bar{\tau}_2)$	4	13.1	I	2	$(A_{4.1}-A_{4.3})$
Pnma	Γ	$P2_1/b,P2_1/m,P2_1/b$		. . .			
	U	$P2_1/m(\tau_1+\tau_5,\tau_4+\tau_8)$	2	C_4	I	2	$A_{2.2}$
		$P2_1/b(\tau_2+\tau_6,\tau_3+\tau_7)$	2	C_4	I	2	$A_{2.2}$
	T	$P2_1/b(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
Cmcm	Γ	$B2/m,B2/b,P2_1/m$		. . .			
	S	$P2_1/m(\tau_1,\tau_4)P2_1/b(\tau_2,\tau_3)$	2	C_{4v}	I	2	$A_{2.1}$
Cmca	Γ	$B2/m,B2/m,P2_1/b$		. . .			
Cmmm	Γ	$B2/m,B2/m,P2/m$		. . .			
	R	$B2/m,(\tau_1,\tau_3)B2/b(\tau_2,\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	S	$P2/m(\tau_1,\tau_4)P2/b(\tau_2,\tau_3)$	2	C_{4v}	I	2	$A_{2.1}$
Cccm	Γ	$B2/b,B2/b,P2/m$		. . .			
	R	$B2/m(\tau_1,\tau_3)B2/b(\tau_2,\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	S	$P2/m(\tau_1,\tau_4)P2/b(\tau_2,\tau_3)$	2	C_{4v}	I	2	$A_{2.1}$
Cmma }	Γ	{ $B2/m,B2/b,P2/b$		. . .			
Ccca }		{ $B2/b,B2/b,P2/b$		. . .			
Fmmm	Γ	$B2/m,B2/m,B2/m$		. . .			
	R	$[P\bar{1},B2/m](\tau_1)[P\bar{1},B2/b](\tau_2)$	4 }	56.1	I,II	2,2	$A_{4.1},A'_{4.1}$
		$[B2/m,B2/m](\tau_1)[B2/b,B2/b](\tau_2)$	4 }		III,IV	4,4	$A''_{4.1},A'''_{4.1}$
Fddd	Γ	$B2/b,B2/b,B2/b$		. . .			
	R	$[P\bar{1},B2/b](\tau_1,\tau_2)$ }	4	82.01	I,II	2,2	$A_{4.1},A'_{4.1}$
		$[B2/b,B2/b](\tau_1,\tau_2)$ }			III,IV	4,4	$A''_{4.1},A'''_{4.1}$
Immm	Γ	$B2/m,B2/m,B2/m$		. . .			
	U	$B2/m(\tau_1,\tau_4)B2/b(\tau_2,\tau_3)$	2	C_{4v}	I	2	$A_{2.1}$
	S	$B2/m(\tau_1,\tau_4)B2/b(\tau_2,\tau_3)$	2	C_{4v}	I	2	$A_{2.1}$
	T	$B2/m(\tau_1,\tau_4)B2/b(\tau_2,\tau_3)$	2	C_{4v}	I	2	$A_{2.1}$
Ibam	Γ	$B2/b,B2/b,B2/m$		. . .			
	S	$B2/m(\tau_1,\tau_4)B2/b(\tau_2,\tau_3)$	2	C_{4v}	I	2	$A_{2.1}$
Ibca	Γ	$B2/b,B2/b,B2/b$		. . .			
Imma	Γ	$B2/m,B2/m,B2/b$		. . .			
	U	$B2/m(\tau_1,\tau_4)B2/b(\tau_2,\tau_3)$	2	C_{4v}	I	2	$A_{2.1}$
	T	$B2/m(\tau_1,\tau_4)B2/b(\tau_2,\tau_3)$	2	C_{4v}	I	2	$A_{2.1}$

TABLE VII. Ferroelastic transitions with a tetragonal high-symmetry phase. Same conventions as Table VI. Whenever ambiguous, the orientation of the LS phases is only indicated once for each Bravais lattice and point-symmetry change (in general, for the first HS group of each class).

HS group	BZ point	Low-symmetry phase	OP dim	(a)	(b)	(c)	(d)
$P4$	Γ	$P2(\tau_2)$	1	C_i	I	1	proper
	R	$B2(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$P2(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_1$	Γ	$P2_1$		. . .			
	X	$P2_1(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_2$	Γ	$P2$		. . .			
	R	$B2(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$P2(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_3$	Γ	$P2_1$		. . .			
	X	$P2_1(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
$I4$	Γ	$B2$		. . .			
	N	$B2(\tau_1)$	4	58.01	I	2	$A_{4.1}$
	X	$B2(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
$I4_1$	Γ	$B2$		. . .			
	Z	$P2_1(\tau_3+\tau_4)$	2	C_4	I	2	$A_{2.2}$
	X	$B2(\tau_1,\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	N	$[B2,B2](\tau_1)$	4	59.1	II,IV	4,8	$A_{4.1},A_{4.2}$
$P4/m$	Γ	$P2/m(\tau_2)$	1	C_i	I	1	proper
		$P\bar{1}(\tau_3+\tau_4)$	2	C_4	I	2	proper
	M	$P2/m(\tau_7+\tau_8)P2/b(\tau_3+\tau_4)$	2	C_4	I	2	$A_{2.2}$
	Z	$P2_1/m(\tau_3+\tau_4,\tau_7+\tau_8)$	2	C_4	I	2	$A_{2.2}$
	A	$B2/m(\tau_3+\tau_4,\tau_7+\tau_8)$	2	C_4	I	2	$A_{2.2}$
	R	$B2/m(\tau_1,\tau_2,\tau_3,\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$P2/m(\tau_1,\tau_4)P2/b(\tau_2,\tau_3)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_2/m$	Γ	$P2/m,P\bar{1}$					
	M	$P2/m(\tau_7+\tau_8)P2/b(\tau_3+\tau_4)$	2	C_4	I	2	$A_{2.2}$
	Z	$P2_1/m(\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	A	$B2/m(\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	R	$B2/m(\tau_1,\tau_2,\tau_3,\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$P2/m(\tau_1,\tau_4)P2/b(\tau_2,\tau_3)$	2	C_{4v}	I	2	$A_{2.1}$
$P4/n$	Γ	$P2/b,P\bar{1}$		. . .			
	M	$P2/b(\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$P2_1/b(\tau_3+\tau_4,\tau_7+\tau_8)$	2	C_4	I	2	$A_{2.2}$
	A	$B2/b(\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_2/n$	Γ	$P2/b,P\bar{1}$		. . .			
	M	$P2/b(\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$P2_1/b(\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	A	$B2/b(\tau_3+\tau_4,\tau_7+\tau_8)$	2	C_4	I	2	$A_{2.2}$
$I4/m$	Γ	$B2/m,P\bar{1}$		. . .			
	Z	$P2_1/m(\tau_7+\tau_8)P2_1/b(\tau_3+\tau_4)$	2	C_4	I	2	$A_{2.2}$
	X	$B2/m(\tau_1,\tau_2)B2/b(\tau_3,\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	N	$[B2/m,P\bar{1}](\tau_1,\tau_2)$	4	58.01	I,IV	2,8	
$I4_1/a$	Γ	$B2/b,P\bar{1}$		. . .			
	Z	$P2_1/b(\tau_2)$	2	C_{4v}	I	2	
	N	$\left.\begin{matrix}[P\bar{1},P\bar{1}]\\ B2/b\end{matrix}\right\}(\tau_1,\tau_2)$	4	80.01	I,III II	2,4 4	$A_{4.1},A_{4.1}$ $A_{4.1}$
$P\bar{4}2m$	Γ	$P222(\tau_2)$	1	C_i	I	1	proper
	M	$C222(\tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$P222_1(\tau_5)$	2	C_{4v}	I	2	$A_{2.1}$

TABLE VII. *(Continued)*

HS group	BZ point	Low-symmetry phases	OP dim	(a)	(b)	(c)	(d)
$P\bar{4}2m$	A	$F222(\tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
	R	$C222(\tau_1, \tau_2, \tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$P222(\tau_1, \tau_3)P222_1(\tau_2, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$P\bar{4}2c$	Γ	$P222$		. . .			
	M	$C222(\tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$P222_1(\tau_2+\tau_4, \tau_3+\tau_5)$	2	C_4	I	2	$A_{2.2}$
	A	$F222(\tau_2+\tau_4, \tau_3+\tau_5)$	2	C_4	I	2	$A_{2.2}$
	R	$C222(\tau_1, \tau_2, \tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$P222(\tau_1, \tau_3)P222_1(\tau_2, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$P\bar{4}2_1m$	Γ	$P2_12_12$					
	Z	$P2_12_12_1(\tau_5)$	2	C_{4v}	I	2	$A_{2.2}$
$P\bar{4}2_1c$	Γ	$P2_12_12$		. . .			
	Z	$P2_12_12_1(\tau_2+\tau_4, \tau_3+\tau_5)$	2	C_4	I	2	$A_{2.2}$
$P\bar{4}m2$	Γ	$C222$					
	M	$P222_1(\tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$C222_1(\tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
	A	$I222(\tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
$P\bar{4}c2$	Γ	$C222$		. . .			
	M	$P2_122(\tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$C222_1(\tau_2+\tau_5, \tau_3+\tau_4)$	2	C_4	I	2	$A_{2.2}$
	A	$I222(\tau_2+\tau_5, \tau_3+\tau_4)$	2	C_4	I	2	$A_{2.2}$
$P\bar{4}b2$	Γ	$C222$		. . .			
	M	$P2_12_12(\tau_2+\tau_5, \tau_3+\tau_4)$	2	C_4	I	2	$A_{2.2}$
	Z	$C222_1(\tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
	A	$I2_12_12_1(\tau_2+\tau_5, \tau_3+\tau_4)$	2	C_4	I	2	$A_{2.2}$
	Γ	$C222$					
$P\bar{4}n2$	M	$P2_12_12(\tau_2+\tau_5, \tau_3+\tau_4)$	2	C_4	I	2	$A_{2.2}$
	Z	$C222_1(\tau_2+\tau_5, \tau_3+\tau_4)$	2	C_4	I	2	$A_{2.2}$
	A	$I2_12_12_1(\tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
	Γ	$F222$		. . .			
$I\bar{4}m2$	Z	$C222_1(\tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$C222(\tau_1, \tau_2)C222_1(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	Γ	$F222$		. . .			
$I\bar{4}c2$	Z	$C222_1(\tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$C222(\tau_1, \tau_2)C222_1(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	Γ	$I222$		. . .			
$I\bar{4}2m$	Z	$P2_12_12(\tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
	N	$C222(\tau_1, \tau_2)$	4	82.01	I	2	$A_{4.1}$
	Γ	$I2_12_12_1$					
$I\bar{4}2d$	Z	$P222_1(\tau_2+\tau_4)$	2	C_4	I	2	$A_{2.2}$
		$P2_12_12_1(\tau_3+\tau_5)$	2	C_4	I	2	$A_{2.2}$
	N	$C222_1(\tau_1, \tau_2)$	4	80.01	III	4	$A_{4.1}$
$P422$	Γ	$P2^x22(\tau_3)C2^{xy}22(\tau_4)$	2	C_i	I	1	proper
	R	$C2^x22(\tau_1, \tau_2, \tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$P2^x22(\tau_1, \tau_3)P222_1(\tau_2, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$P42_12$	Γ	$P2_12_12, C222$		. . .			
	M	$P2^{xy}22(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
		$P2_122(\tau_2+\tau_3, \tau_4+\tau_5)$	2	C_4	I	2	$A_{2.2}$
	A	$I2^{xy}22(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
		$I2_12_12_1(\tau_2+\tau_3, \tau_4+\tau_5)$	2	C_4	I	2	$A_{2.2}$
$P4_122$	Γ	$P222_1, C222_1$		. . .			
$P4_322$	X	$P222_1(\tau_1, \tau_3)P2_12_12(\tau_2, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_12_12$	Γ	$P2_12_12_1, C222_1$		. . .			
$P4_32_12$	M	$P222_1(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$

TABLE VII. *(Continued)*

HS group	BZ point	Low-symmetry phases	OP dim	(a)	(b)	(c)	(d)
$P4_32_12$	M	$P2_12_12(\tau_2+\tau_3,\tau_4+\tau_5)$	2	C_4	I	2	$A_{2.2}$
$P4_222$	Γ	$P222,C222$					
	R	$C222(\tau_1,\tau_2,\tau_3,\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$P222(\tau_1,\tau_3)P222_1(\tau_2,\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_22_12$	Γ	$P2_12_12,C222$		. . .			
	M	$P222(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
		$P2_122(\tau_2+\tau_3,\tau_4+\tau_5)$	2	C_4	I	2	$A_{2.2}$
	A	$I2_12_12_1(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
		$I222(\tau_2+\tau_3,\tau_4+\tau_5)$	2	C_4	I	2	$A_{2.2}$
$I422$	Γ	$I2^x22,F2^{xy}22$					
	X	$C2^{xy}22(\tau_1,\tau_4)C222_1(\tau_2,\tau_3)$	2	C_{4v}	I	2	$A_{2.1}$
	N	$C2^x22(\tau_1,\tau_2)$	4	82.01	I	4	$A_{4.1}$
$I4_122$	Γ	$I2_12_12_1,F222$					
	X	$C222(\tau_1,\tau_4)C222(\tau_2,\tau_3)$	2	C_{4v}	I	2	$A_{2.1}$
	N	$\left.\begin{matrix}C222_1\\I222\end{matrix}\right\}(\tau_1,\tau_2)$	4	80.01	I	4	$A_{4.1}$
					III	8	$A_{4.1}$
$P4mm$	Γ	$Pm^xm2(\tau_3)Cm^{xy}m2(\tau_4)$	1	C_i	I	1	proper
	M	$[Cm^xm2,Pm^{xy}a2](\tau_5)$	2	C_{4v}	I,II	2,2	$A_{2.1},A_{2.1}$
	Z	$[Pm^xc2_1,Cm^{xy}c2_1](\tau_5)$	2	C_{4v}	I,II	2,2	$A_{2.1},A_{2.1}$
	A	$[Fm^xm2,Im^{xy}a2](\tau_5)$	2	C_{4v}	I,II	2,2	$A_{2.1},A_{2.1}$
	R	$Am^xm2(\tau_1,\tau_4)Abm2(\tau_2,\tau_3)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$Pm^xm2(\tau_1,\tau_2)Pma2(\tau_3,\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$P4bm$	Γ	$Pba2,Cmm2$					
	M	$Pma2(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$[Pna2_1,Cmc2_1](\tau_5)$	2	C_{4v}	I,II	2,2	$A_{2.1},A_{2.1}$
	A	$Ima2(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_2cm$	Γ	$Pcc2,Cmm2$		. . .			
	M	$[Cmm2,Pma2](\tau_5)$	2	C_{4v}	I,II	2,2	$A_{2.1},A_{2.1}$
	Z	$Cmc2_1(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
	A	$Iba2(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$Pcc2(\tau_1,\tau_2)Pnc2(\tau_3,\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_2nm$	Γ	$Pnn2,Cmm2$		. . .			
	M	$Pma2(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$Cmc2_1(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
	A	$[Fdd2,Ima2](\tau_5)$	2	C_{4v}	I,II	2,2	$A_{2.1},A_{2.1}$
$P4cc$	Γ	$Pcc2,Ccc2$		. . .			
	M	$[Cmm2,Pma2](\tau_5)$	2	C_{4v}	I,II	2,2	$A_{2.1},A_{2.1}$
	X	$Pcc2(\tau_1,\tau_2)Pnc2(\tau_3,\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$P4nc$	Γ	$Pnn2,Ccc2$					
	M	$Pma2(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
	A	$Fdd2(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_2mc$	Γ	$Pmm2,Ccc2$		. . .			
	M	$[Cmm2,Pma2](\tau_5)$	2	C_{4v}	I,II	2,2	$A_{2.1},A_{2.1}$
	Z	$Pmc2_1(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
	A	$Fmm2(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
	R	$Amm2(\tau_1,\tau_2)Abm2(\tau_3,\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$Pmm2(\tau_1,\tau_2)Pma2(\tau_3,\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_2bc$	Γ	$Pba2,Ccc2$		. . .			
	M	$Pma2(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$Pna2_1(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$

TABLE VII. *(Continued)*

HS group	BZ point	Low-symmetry phases	OP dim	(a)	(b)	(c)	(d)
$I4mm$	Γ	$\mathrm{Im}^{x}m2, Fm^{xy}m2$		. . .			
	Z	$[Pm^{x}n2_1, Cm^{xy}c2_1](\tau_5)$		C_{4v}	I,II	2,2	$A_{2.1}, A_{2.1}$
	X	$Am^{xy}m2(\tau_1)Ama2(\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
		$Aba2(\tau_3)Abm2(\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	N	$Am^{x}m2(\tau_1)Abm2(\tau_2)$	4	82.01	I	4	$A_{4.1}$
	A	$[Im^{x}a2, Fd^{xy}d2](\tau_2, \tau_4)$	4	26.1	I,II	4,4	$A_{4.1}, A_{4.3}$
$I4cm$	Γ	$Iba2, Fmm2$		. . .			
	Z	$[Pca2_1, Cmc2_1](\tau_5)$	2	C_{4v}	I,II	2,2	$A_{2.1}, A_{2.1}$
	X	$Ama2(\tau_1)Amm2(\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
		$Abm2(\tau_3)Aba2(\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$I4_1md$	Γ	$Imm2, Fdd2$		. . .			
	Z	$Pmn2_1(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
	N	$Amm2(\tau_1)Abm2(\tau_2)$ }	4	80.01	I	4	$A_{4.1}$
		$Imm2(\tau_1)Iba2(\tau_3)$ }			III	8	$A_{4.1}$
$I4_1cd$	Γ	$Iba2, Fdd2$		. . .			
	Z	$Pca2_1(\tau_1)$	2	C_{4v}	I	2	$A_{2.1}$
$P4/mmm$	Γ	$Pm^{x}ma(\tau_3)Cm^{xy}cm(\tau_4)$	I	C_i	I	1	proper
		$[P2^{x}/m, B2^{xy}/m](\tau_5)$	2	C_{4v}	I,II	2,2	proper
	M	$[Cm^{x}ma, Pb^{xy}am](\tau_5)[Cmmm, Pmma](\tau_{10})$	2	C_{4v}	I,II	2,2	$A_{2.1}, A_{2.1}$
	A	$[Fm^{x}mm, \mathrm{Im}^{xy}ma](\tau_5, \tau_{10})$	2	C_{4v}	I,II	2,2	$A_{2.1}, A_{2.1}$
	Z	$[Pm^{x}maCm^{xy}cm](\tau_5, \tau_{10})$	2	C_{4v}	I,II	2,2	$A_{2.1}, A_{2.1}$
	R	$Cm^{x}mm(\tau_1, \tau_2, \tau_7, \tau_8)Cmcm(\tau_3, \tau_4, \tau_5, \tau_6)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$Pm^{x}mm(\tau_1, \tau_7)Pmma(\tau_2, \tau_4, \tau_6, \tau_8)Pbam(\tau_3, \tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
$P4/mcc$	Γ	$Pccm, Cccm, P2/c, B2/m$		. . .			
	X	$Pccm(\tau_1, \tau_7)Pcca(\tau_2, \tau_4, \tau_6, \tau_8)Pban(\tau_3, \tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
$P4/nbm$	Γ	$Pban, Cmma, P2/b, B2/m$		. . .			
	M	$Pccm(\tau_1)Pmma(\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	A	$Ibam(\tau_1, \tau_2)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$[Pnna, Cmca](\tau_5, \tau_{10})$	2	C_{4v}	I,II	2,2	$A_{2.1}, A_{2.1}$
$P4/nnc$	Γ	$Pnnn, Ccca, P2/b, B2/b$		. . .			
	M	$Pban(\tau_3)Pbcn(\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	A	$Fddd(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$P4/mbm$	Γ	$Pbam, Cmmm, P2_1/b, B2/b$		. . .			
	M	$Pmma(\tau_1)Pmna(\tau_6)$	2	C_{4v}	I	2	$A_{2.1}$
		$Pban(\tau_2+\tau_5)Pmmn(\tau_3+\tau_4)Pbam(\tau_7, \tau_{10})Pmmm(\tau_8+\tau_9)$	2	C_4	I	2	$A_{2.2}$
	A	$Imma(\tau_1)Ibam(\tau_6)$	2	C_{4v}	I	2	$A_{2.1}$
		$Imma(\tau_3+\tau_4, \tau_8+\tau_9)Ibam(\tau_2+\tau_5, \tau_7+\tau_{10})$	2	C_4	I	2	$A_{2.2}$
	Z	$[Pnma, Cmcm](\tau_5, \tau_{10})$	2	C_{4v}	I,II	2,2	$A_{2.1}, A_{2.1}$
$P4/mnc$	Γ	$Pnnm, Cccm, P2_1/b, B2/b$		. . .			
	M	$Pmna(\tau_1)Pnna(\tau_6)$	2	C_{4v}	I	2	$A_{2.1}$
		$Pnnn(\tau_2+\tau_5)Pccn(\tau_3+\tau_4)Pnnm(\tau_7+\tau_{10})Pccm(\tau_8+\tau_9)$	2	C_4	I	2	$A_{2.2}$
	R	$\left.\begin{array}{l} B2^{z}/m \\ Fd^{xy}dd \\ P2_1^{x}/b, B2^{xy}/b \end{array}\right\}(\tau_1, \tau_2)$			I	2	$(A_{4.1} - A'_{4.1})$
			4	58.01	IV	4	$A_{4.1}$
					II,V	2,4	$E_{4.5}, E_{4.5}$
$P4/nmm$	Γ	$Pmmn, Cmma, P2_1/m, B2/m$		. . .			
	M	$Pbam(\tau_3)Pccm(\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	A	$Ibam(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$[Pnma, Cmca](\tau_5, \tau_{10})$	2	C_{4v}	I,II	2,2	$A_{2.1}, A_{2.1}$
$P4/ncc$	Γ	$Pccn, Ccca, P2_1/b, B2/b$		. . .			
	M	$Pbcn(\tau_1)Pban(\tau_2)$	2	C_{4v}	I	2	$A_{2.1}$

TABLE VII. *(Continued)*

HS group	BZ point	Low-symmetry phases	OP dim	(a)	(b)	(c)	(d)
$P4_2/mmc$	Γ	$Pmmm, Cccm, P2/m, B2/b$		. . .			
	M	$[Cmma, Pnna](\tau_5)[Cmmm, Pmna](\tau_{10})$	2	C_{4v}	I,II	2,2	$A_{2.1}, A_{2.1}$
	A	$Fmmm(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$Pmma(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	R	$Cmmm(\tau_1, \tau_2, \tau_7, \tau_8)Cmcm(\tau_3, \tau_4, \tau_5, \tau_6)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$Pmmm(\tau_1, \tau_7)Pmma(\tau_2, \tau_4, \tau_6, \tau_8)Pbam(\tau_3, \tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_2/mcm$	Γ	$Pccm, Cmmm, P2/b, B2/m$		. . .			
	M	$[Ccca, Pbam](\tau_5)[Cccm, Pmma](\tau_{10})$	2	C_{4v}	I,II	2,2	$A_{2.1}, A_{2.1}$
	A	$Immm(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$Cmcm(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	X	$Pccm(\tau_1, \tau_7)Pcca(\tau_2, \tau_4, \tau_6, \tau_8)$	2	C_{4v}	I	2	$A_{2.1}$
		$Pban(\tau_3, \tau_5)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_2/nbc$	Γ	$Pban, Ccca, P2/b, B2/b$		. . .			
	M	$Pban(\tau_3)Pbcn(\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$Pnna(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_2/nnm$	Γ	$Pnnn, Cmma, P2/b, B2/b$		. . .			
	M	$Pcca(\tau_3)Pnma(\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	A	$[Fddd, Ibam](\tau_5, \tau_{10})$	2	C_{4v}	I,II	2,2	$A_{2.1}, A_{2.1}$
	Z	$Cmca(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_2/mbc$	Γ	$Pbam, Cccm, P2_1/b, B2/b$		. . .			
	M	$Pmna(\tau_1)Pnna(\tau_6)$	2	C_{4v}	I	2	$A_{2.1}$
		$Pnnn(\tau_2+\tau_5)Pccn(\tau_3+\tau_4)Pnnm(\tau_7+\tau_{10})Pccm(\tau_8+\tau_9)$	2	C_4	I	2	$A_{2.2}$
	Z	$Pnma(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_2/mnm$	Γ	$Pnnm, Cmmm, P2_1/b, B2/m$		. . .			
	M	$Pmma(\tau_1)Pmna(\tau_6)$	2	C_{4v}	I	2	$A_{2.1}$
		$Pban(\tau_2+\tau_5)Pmmn(\tau_3+\tau_4)Pbam(\tau_7+\tau_{10})Pmmm(\tau_8+\tau_9)$	2	C_4	I	2	$A_{2.2}$
	A	$Imma(\tau_1, \tau_2)Ibam(\tau_4)Immm(\tau_3)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$Cmcm(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
		$B2^z/m$					
	R	$Fm^{xy}mm \; \}(\tau_1, \tau_2)$	4	58.01	I	2	$(A_{4.1} - A'_{4.1})$
		$P2_1^x/b, B2^{xy}/m$			IV	4	$A_{4.1}$
					II,V	2,4	$E_{4.5}, E_{4.5}$
$P4_2/nmc$	Γ	$Pmmn, Ccca, P2_1/m, B2/b$		. . .			
	M	$Pbcn(\tau_3)Pban(\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	Z	$Pmma(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$P4_2/ncm$	Γ	$Pccn, Cmma, P2_1/b, B2/b$		. . .			
	M	$Pbam(\tau_3)Pccm(\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	A	$Ibam(\tau_1, \tau_6)$	2	C_{4v}	I	2	$A_{2.1}$
		$Imma(\tau_2+\tau_4, \tau_8+\tau_{10})Ibca(\tau_3+\tau_5, \tau_7+\tau_9)$	2	C_4	I	I	$A_{2.2}$
	Z	$Cmca(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
$I4/mmm$	Γ	$\mathrm{Im}^x mm, Fm^{xy}mm, B2^x/m, B2^{xy}/m$		. . .			
	Z	$[Pn^xnm, Cm^{xy}ca](\tau_5)[Pnmm, Cmcm](\tau_{10})$	2	C_{4v}	I,II	2,2	$A_{2.1}, A_{2.1}$
	X	$Cm^{xy}mm(\tau_1)Cccm(\tau_2)Cmca(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
		$Ccca(\tau_5)Cmma(\tau_6)Cmcm(\tau_7, \tau_8)$	2	C_{4v}	I	2	$A_{2.1}$
	N	$[Cm^xmm, B2^x/m](\tau_1, \tau_4)[Cmca, B2/b](\tau_2, \tau_3)$ }	4	82.01	II,I	4,2	$A_{4.1}, E_{4.5}$
		$B2^{xy}/m(\tau_1, \tau_4)B2/b(\tau_2, \tau_3)$ }			V	4	$E_{4.5}$
$I4/mcm$	Γ	$Ibam, Fmmm, B2/b, B2/m$		. . .			
	Z	$[Pbcn, Cmca](\tau_5)[Pbcm, Cmcm](\tau_{10})$	2	C_{4v}	I,II	2,2	$A_{2.1}, A_{2.1}$
	X	$Cmma(\tau_1)Ccca(\tau_2)Cmcm(\tau_3, \tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
		$Cccm(\tau_5)Cmmm(\tau_6)Cmca(\tau_7, \tau_8)$	2	C_{4v}	I	2	$A_{2.1}$
$I4_1/amd$	Γ	$Imma, Fddd, B2/m, B2/b$		. . .			
	Z	$Pnma(\tau_3)Pmna(\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$
	N	$[Cmmm, B2/m](\tau_1, \tau_4)[Cmca, B2/b](\tau_2, \tau_3)$ }	4	101.01	II,I	4,2	$A_{4.1}, E_{4.4}$
		$B2/b(\tau_1, \tau_2, \tau_3, \tau_4)$ }			III	4	$E_{4.4}$
$I4_1/acd$	Γ	$Ibca, Fddd, B2/b, B2/b$		. . .			
	Z	$Pbca(\tau_3)Pcca(\tau_4)$	2	C_{4v}	I	2	$A_{2.1}$

TABLE VIII. Ferroelastic transitions with a trigonal or hexagonal high-symmetry phase. Same conventions as Table VII.

HS group	BZ point	Low-symmetry phases	OP dim	(a)	(b)	(c)	(d)
$P\bar{3}$	A	$P\bar{1}(\tau_2+\tau_3,\tau_5+\tau_6)$	2	C_6	I	2	$E_{2.1}$
$R\bar{3}$	M	$P\bar{1}(\tau_2)$	3	T_h	I	2	$E_{3.1}$
	L	$P\bar{1}(\tau_1,\tau_2)$					
$P\bar{3}1m$	A	$[B2/m,B2/b](\tau_3,\tau_6)$	2	C_{6v}	I,II	2,2	$E_{2.1};E_{2.1}$
$P\bar{3}m1$	M	$P2_1/b(\tau_2)$	3	O	I	2	$E_{3.1}$
		$P2/b(\tau_3)P2_1/m(\tau_4)$	3	O_h	I	2	$E_{3.1}$
	L	$B2/m(\tau_1,\tau_4)B2/b(\tau_2,\tau_3)$					
$P\bar{3}1c$	M	$P2_1/b(\tau_2)$	3	O	I	2	$E_{3.1}$
$P\bar{3}c1$		$P2_1/b(\tau_4)P2/b(\tau_3)$	3	O_h	I	2	$E_{3.1}$
$R\bar{3}m$	A	$[B2/m,B2/b](\tau_3,\tau_6)$	2	C_{6v}	I,II	2,2	$E_{2.1};E_{2.1}$
	M	$P2_1/m(\tau_4)P2/c(\tau_3)$	3	O_h	I	2	$E_{3.1}$
		$P2_1/c(\tau_2)$	3	O	I	2	$E_{3.1}$
	L	$B2/m(\tau_1,\tau_4)B2/b(\tau_2,\tau_3)$	3	O_h	I	2	$E_{3.1}$
$R\bar{3}c$	X	$P2_1/c(\tau_2)$	3	O	I	2	$E_{3.1}$
		$P2_1/c(\tau_4)P2/c(\tau_3)$	3	O_h	I	2	$E_{3.1}$
$P6$	M	$P2(\tau_2)$	3	T_h	I	2	$E_{3.1}$
$P6_2$	L	$B2(\tau_2)$					
$P6_4$							
$P6_1$	M	$P2_1(\tau_2)$					
$P6_3$							
$P6_5$							
$P6/m$	Γ	$P\bar{1}(\tau_{11}+\tau_{12})$	2	C_6	I	1	proper
	A	$P2/m(\tau_3+\tau_4,\tau_9+\tau_{10})$	2	C_6	I	2	$E_{2.1}$
		$P2_1/m(\tau_5+\tau_6,\tau_{11}+\tau_{12})$					
	M	$P2/m(\tau_4)P2/b(\tau_2,\tau_3)$	3	T_h	I	2	$E_{3.1}$
	L	$B2/m(\tau_1,\tau_2,\tau_3,\tau_4)$					
$P6_3/m$	Γ	$P\bar{1}$		...			
	M	$P2_1/m(\tau_4)P2_1/b(\tau_2,\tau_3)$	3	T_h	I	2	$E_{3.1}$
$P622$	M	$P2_12_12(\tau_4)$	3	O	I	2	$E_{3.1}$
$P6_222$		$P222_1(\tau_2,\tau_3)$	3	O_h	I	2	$E_{3.1}$
$P6_422$	L	$I222(\tau_1,\tau_4)$					
		$I2_12_12_1(\tau_2,\tau_3)$					
$P6_122$							
$P6_522$	M	$P2_12_12_1(\tau_4)$	3	O	I	2	$E_{3.1}$
$P6_322$		$P2_12_12(\tau_2,\tau_3)$	3	O_h	I	2	$E_{3.1}$
$P6mm$	A	$[CmC2_1,Cmc2_1](\tau_5)$	2	C_{6v}	I,II	2,2	$E_{2.1},E_{2.1}$
		$[Ccc2,Cmm2](\tau_6)$	2	C_{6v}	I,II	2,2	$E_{2.1},E_{2.1}$
	M	$Pba2(\tau_3)$	3	O	I	2	$E_{3.1}$
	L	$Pma2(\tau_2,\tau_4)$	3	O_h	I	2	$E_{3.1}$
		$Imm2(\tau_1)Iba2(\tau_3)$					
		$Ima2(\tau_2,\tau_4)$					
$P6cc$	M	$Pnn2(\tau_3)$	3	O	I	2	$E_{3.1}$
		$Pnc2(\tau_2,\tau_4)$	3	O_h	I	2	$E_{3.1}$
$P6_3cm$	M	$Pna2_1(\tau_3)$	3	O	I	2	$E_{3.1}$
		$Pmn2_1(\tau_2)Pca2_1(\tau_4)$	3	O_h	I	2	$E_{3.1}$
$P6_3mc$	M	$Pna2_1(\tau_3)$	3	O	I	2	$E_{3.1}$
		$Pca2_1(\tau_2)Pmn2_1(\tau_4)$	3	O_h	I	2	$E_{3.1}$
$P6/mmm$	Γ	$[B2^x/m,B2^x/m](\tau_5)$	2	C_{6v}	I,II	1,1	proper
		$C222(\tau_{12})$	2	C_{6v}	I	1	$E_{2.1}$
	A	$[Cccm,Cmmm](\tau_6,\tau_{12})$	2	C_{6v}	I,II	2,2	$E_{2.1},E_{2.1}$
		$[Cmcm,Cmcm](\tau_5,\tau_{11})$	2	C_{6v}	I,II	2,2	$E_{2.1},E_{2.1}$
	M	$Pbam(\tau_4)$	3	O	I	2	$E_{3.1}$

TABLE VIII. *(Continued)*

HS group	BZ point	Low-symmetry phases	OP dim	(a)	(b)	(c)	(d)
$P6/mmm$	M	$Pmna(\tau_2,\tau_3)Pban(\tau_5)$ $Pmma(\tau_6,\tau_7)Pmmn(\tau_8)$	3	O	I	2	$E_{3.1}$
	L	$Immm(\tau_1,\tau_8)Ibam(\tau_4,\tau_5)$ $Imma(\tau_2,\tau_3,\tau_6,\tau_7)$	3	O_h	I	2	$E_{3.1}$
$P6/mcc$	Γ	$B2/b,B2/b,C222$		. . .			
	M	$Pnnm(\tau_4)$	3	O	I	2	$E_{3.1}$
		$Pnna(\tau_2,\tau_3)Pnnn(\tau_5)$ $Pmna(\tau_6,\tau_7)Pccn(\tau_8)$	3	O_h	I	2	$E_{3.1}$
$P6_3/mcm$	Γ	$B2/b,B2/m,C222_1$		. . .			
	M	$Pnma(\tau_4)$	3	O	I	2	$E_{3.1}$
		$Pnnm(\tau_2)Pbcn(\tau_3)$ $Pnna(\tau_5)Pbcm(\tau_6)$ $Pmmn(\tau_7)Pnma(\tau_8)$	3	O_h	I	2	$E_{3.1}$
$P6_3/mmc$	Γ	$B2/m,B2/b,C222_1$		. . .			
	M	$Pnma(\tau_4)$	3	O	I	2	$E_{3.1}$
		$Pbcn(\tau_2)Pnnm(\tau_3)$ $Pnna(\tau_5)Pmmn(\tau_6)$ $Pbcm(\tau_7)Pnma(\tau_8)$	3	O_h	I	2	$E_{3.1}$

TABLE IX. Ferroelastic transition with a cubic high-symmetry phase. Same conventions as Table VII.

HS group	BZ point	Low-symmetry phases	OP dim	(a)	(b)	(c)	(d)
$P23$	R	$F222(\tau_2+\tau_3)$	2	C_6	I	2	$E_{2.1}$
	X	$P222(\tau_1,\tau_2)P222_1(\tau_3,\tau_4)$	3	T_h	I	2	$E_{3.1}$
$F23$		No continuous *PFT* transitions					
$I23$	H	$P222(\tau_2+\tau_3)$	2	C_6	I	2	$E_{2.1}$
	P	$F222(\tau_2+\tau_3)$	2	C_{12}	I	4	$E_{2.2}$
$P2_13$		No continuous transitions					
$I2_13$	H	$P2_12_12_1(\tau_2+\tau_3)$	2	C_6	I	2	$E_{2.1}$
$Pm3$	Γ	$P222(\tau_6,\tau_7)$	2	C_6	I	1	$E_{2.1}$
	R	$Fmmm(\tau_2+\tau_3,\tau_6+\tau_7)$	2	C_6	I	2	$E_{2.1}$
		$[Fmmm,R\bar{3}](\tau_4,\tau_8)$	3	T_h	I,II	2,2	$E_{3.1},T_{3.1}$
	X	$Pmmm(\tau_1,\tau_6)Pccm(\tau_2,\tau_5)$ $Pmma(\tau_3,\tau_4,\tau_7,\tau_8)$	3	T_h	I	2	$E_{3.1}$
	M	$Cmmm(\tau_7,\tau_8)Cmma(\tau_5,\tau_6)$	3	T_h	I	2	$E_{3.1}$
$Pn3$	Γ	$P222$		. . .			
	R	$Fddd(\tau_2+\tau_3,\tau_6+\tau_7)$	2	C_6	I	2	$E_{2.1}$
		$[Fddd,R\bar{3}](\tau_4,\tau_8)$	3	T_h	I,II	2,2	$E_{3.1},T_{3.1}$
$Fm3$	Γ	$F222$		. . .			
	X	$Ccca(\tau_5)Cmcm(\tau_6,\tau_7)Cmma(\tau_8)$	3	T_h	I	2	$E_{3.1}$
	L	$R\bar{3}(\tau_1,\tau_4)$	4	95.1	I	2	$T_{4.1}$
		$P\bar{1}$ $\}(\tau_2+\tau_3,\tau_5+\tau_6)$			I	2	$(E_{8.1}-T_{8.1})$
		$[B2/m,Fmmm]$ $\}(\tau_2+\tau_3,\tau_5+\tau_6)$	8	M_4	II,III	4,8	$T_{8.1},E_{8.1}$

TABLE IX. *(Continued)*

HS group	BZ point	Low-symmetry phases	OP dim	(a)	(b)	(c)	(d)
$Fd3$	Γ	$F222$		. . .			
	L	$R\bar{3}(\tau_1,\tau_4)$	4	108.01	I	2	$T_{4.1}$
		$P\bar{1}$			I	2	$(E_{8.1}-T_{8.1})$
		$[B2/b,F222]$ $(\tau_2+\tau_3,\tau_5+\tau_6)$	8	M_3	II,III	4,8	$T_{8.1}(E_{8.1}-A_{8.1})$
$Im3$	Γ	$I222$		. . .			
	H	$Pmmm(\tau_2+\tau_3)Pnnn(\tau_6+\tau_7)$	2	C_6	I	2	$E_{2.1}$
		$[Pnnm,R\bar{3}](\tau_4)[Pmmn,R\bar{3}](\tau_8)$	3	T_h	I,II	2,2	$E_{3.1},T_{3.1}$
	N	$[B2/b,Cmma](\tau_3)[B2/m,Cmmm](\tau_4)$	6	L_8	I,II	2,4	$T_{6.1},E_{6.1}$
		$[Ibca,R\bar{3}](\tau_3)[Immm,R\bar{3}](\tau_4)$			VI,III	8,8	$E_{6.1},T_{6.1}$
	P	$[F222,Fmmm,Fddd](\tau_2+\bar{\tau}_2,\tau_3+\bar{\tau}_3)$	4	42.1	I,II,III	4,4,4	$E_{4.1},E_{4.2},E_{4.2}$
$Pa3$	Γ	$P2_12_12_1$		. . .			
	R	$P\bar{1}(\tau_1+\bar{\tau}_1,\tau_4+\bar{\tau}_4)$	4	49.1	I	2	$T_{4.2}$
		$R\bar{3}(\tau_2+\bar{\tau}_2,\tau_3+\bar{\tau}_3,\tau_5+\bar{\tau}_5,\tau_6+\bar{\tau}_6)$	4	49.2	I	2	$T_{4.1}$
$Ia3$	Γ	$I2_12_12_1$		. . .			
	H	$Pbca(\tau_2+\tau_3,\tau_6+\tau_7)$	2	C_6	I	2	$E_{2.1}$
		$[Pcca,R\bar{3}](\tau_4,\tau_8)$	3	T_h	I,II	2,2	$E_{3.1},T_{3.1}$
$P432$	R	$[I422,I422](\tau_3)$	2	C_{6v}	I,II	2,2	$E_{2.1},E_{2.1}$
	X	$P422(\tau_1,\tau_2)P4_222(\tau_3,\tau_4)$	3	O_h	I	2	$E_{3.1}$
	M	$P422(\tau_2,\tau_3)$	3	O	I	2	$E_{3.1}$
$P4_232$	R	$[I4_122,I4_122](\tau_3)$	2	C_{6v}	I,II	2,2	$E_{2.1},E_{2.1}$
	X	$P4_122(\tau_2,\tau_3)P4_322(\tau_4,\tau_5)$	3	O_h	I	2	$E_{3.1}$
	M	$P4_222(\tau_3,\tau_4)$	3	O	I	2	$E_{3.1}$
$F432$	X	$P4_122(\tau_2)P4_22_12(\tau_3)$	3	O	I	2	$E_{3.1}$
	L	$R32(\tau_1,\tau_2)$	4	109.01	I	2	$T_{4.1}$
	W	$[I422,I4_122](\tau_1,\tau_4)$	6	L_2	I,II	4,4	$E_{6.1},E_{6.1}$
$F4_132$	X	$P4_12_12(\tau_3)P4_32_12(\tau_4)$	3	O	I	2	$E_{3.1}$
	L	$R32(\tau_1,\tau_2)$	4	110.1	I	2	$T_{4.1}$
$I432$	H	$[P422,P4_222](\tau_3)$	2	C_{6v}	I,II	2	$E_{2.1}$
	N	$[C222_1,P4_222](\tau_3)[C222_1,P42_12](\tau_4)$	6	L_6	I,II	2,4	$T_{6.1},E_{6.1}$
		$[I422,R32](\tau_3)[I4_122,R32](\tau_4)$			VI,III	8,8	$E_{6.1},T_{6.1}$
	P	$[I422,I4_122](\tau_2+\bar{\tau}_2,\tau_3+\bar{\tau}_3)$	2	C_{12v}	I,II	4	$E_{2.2},E_{2.2}$
$P4_332$ $P4_132$		No continuous *PFT* transitions					
$I4_132$	H	$[P4_32_12,P4_12_12](\tau_3)$	2	C_{6v}	I,II	2,2	$E_{2.1},E_{2.1}$
	N	$[C222_1,P4_12_12,R32](\tau_3,\tau_4)$	6	L_5	I,II,III	2,4,8	$T_{6.1},E_{6.1},T_{6.1}$
$P\bar{4}3m$	Γ	$[P\bar{4}(\tau_5)]$	3	O	I	1	$E_{3.1}$
	R	$[I\bar{4}m2,I\bar{4}c2](\tau_3)$	2	C_{6v}	I,II	2,2	$E_{2.1}$
		$I\bar{4}m2(\tau_4)I\bar{4}c2(\tau_5)$	3	O_h	I	2	$E_{3.1}$
	X	$P\bar{4}2m(\tau_1,\tau_4)P\bar{4}2c(\tau_2,\tau_3)$	3	O_h	I	2	$E_{3.1}$
		$P222_1(\tau_5)$			II	2	$(A_{6.1}-E_{6.1})$
		$[P\bar{4}2_1m,P\bar{4}2_1m](\tau_5)$	6	L_7	VI,VII	4,4	$E_{6.1},E_{6.1}$
	M	$P\bar{4}b2(\tau_2,\tau_3)$	3	O	I	2	$E_{3.1}$
$F\bar{4}3m$	Γ	$I\bar{4}$		. . .			
	X	$P\bar{4}n2(\tau_2,\tau_3)$	3	O	I	2	$E_{3.1}$
	L	$[I\bar{4}m2,I\bar{4}c2](\tau_3)$	8	M_2	IV,V	8,8	$E_{8.1}$
	W	$[I\bar{4}2m,I\bar{4}2d](\tau_1,\tau_2)$	6	L_3	I,II	4,4	$E_{6.1},E_{6.1}$
$I\bar{4}3m$	Γ	$I\bar{4}$		. . .			
	H	$[P\bar{4}2m,P\bar{4}2c](\tau_3)$	2	C_{6v}	I,II	2,2	$E_{2.1}$
		$P\bar{4}2m(\tau_4)P\bar{4}2c(\tau_5)$	3	O_h	I	2	$E_{3.1}$
	N	$[P\bar{4}c2,I\bar{4}2m](\tau_3)[P\bar{4}b2,I\bar{4}2d](\tau_4)$	6	L_6	II,VI	4,8	$E_{6.2},E_{6.1}$
	P	$[F222,I\bar{4}m2,I\bar{4}c2](\tau_3+\bar{\tau}_3)$	4	44.1	I,II,III	4,4,4	$E_{4.2},E_{4.2},E_{4.2}$
$P\bar{4}3n$	Γ	$P\bar{4}$		. . .			

TABLE IX. *(Continued)*

HS group	BZ point	Low-symmetry phases	OP dim	(a)	(b)	(c)	(d)
$P\bar{4}3n$	R	$F222(\tau_3+\bar{\tau}_3)$	4	21.1	I	2	$E_{4.3}$
	X	$[P222_1,P\bar{4}2_1c](\tau_2+\tau_4,\tau_3+\tau_5)$	6	L_{10}	I,II	2,2	$(E_{6.3}-A_{6.1})E_{6.3}$
	M	$P\bar{4}n2(\tau_3,\tau_4)$	3	O	I	2	$E_{3.1}$
$F\bar{4}3c$	Γ	$I\bar{4}$		. . .			
	X	$P\bar{4}b2(\tau_3,\tau_4)$	3	O	I	2	$E_{3.1}$
$I\bar{4}3d$	Γ	$I\bar{4}$		. . .			
	H	$P2_12_12_1(\tau_3+\bar{\tau}_3)$	4	21.1	I	2	$E_{4.3}$
	P	$I\bar{4}(\tau_2+\bar{\tau}_2,\tau_3+\bar{\tau}_3)$	4	98.1	I	4	$T_{4.2}$
$Pm3m$	Γ	$[P422,P\bar{4}2m](\tau_8)$	2	C_{6v}	I,II	1,1	$E_{2.1},E_{2.1}$
		$[P4/m,R\bar{3}](\tau_5)$	3	O	I,II	1,1	$E_{2.1},T_{3.1}$
		$[P\bar{4}m2,R32](\tau_9)$	3	O_h	I,II	1,1	$E_{2.1},T_{3.1}$
	R	$[I4/mmm,I4/mcm](\tau_3,\tau_8)$	2	C_{6v}	I,II	2,2	$E_{2.1},E_{2.1}$
		$[I4/mmm,R\bar{3}m](\tau_4,\tau_9)[14/mcm,R\bar{3}c](\tau_5,\tau_{10})$	3	O_h	I,II	2,2	$E_{3.1},T_{3.1}$
	X	$P4/mmm(\tau_1,\tau_7)P4/mcc(\tau_2,\tau_6)$	3	O_h	I	2	$E_{3.1}$
		$P4_2/mmc(\tau_3,\tau_9)P4_2/mcm(\tau_4,\tau_8)$					
		$[Cmcm,Pmma](\tau_5,\tau_{10})$	6	L_7	I,II	2,2	$T_{6.1},(E_{6.1}-A_{6.2})$
		$[P4/nmm,P4/mbm](\tau_5)[P4/mbm,P4/nmm](\tau_{10})$			VI,VII	4,4	$E_{6.1},E_{6.1}$
		$[R\bar{3}c,R\bar{3}m](\tau_5)[R\bar{3}m,R\bar{3}c](\tau_{10})$			III,IV	8,8	$T_{6.1},T_{6.1}$
	M	$P4/mbm(\tau_2,\tau_3)$	3	O	I	2	$E_{3.1}$
		$P4/nbm(\tau_6,\tau_9)P4/nmm(\tau_7,\tau_8)$	3	O_h	I	2	$E_{3.1}$
		$[Pmma,Cmmm]$ (τ_{10})	6	L_7	I,II	2,2	$T_{6.1},(E_{6.1},A_{6.2})$
		$[I4/mmm,I4/mmm,R32]$			VI,VII,IV	4,4	$T_{6.2},E_{6.1}$
						4	$E_{6.1}$
$Pn3n$	Γ	$P422,P\bar{4}2c,P4/n,R\bar{3},P\bar{4}n2,R32$		. . .			
	R	$[Fddd,I422](\tau_3+\bar{\tau}_3,\tau_4+\bar{\tau}_4)$	4	48.1	I,II	2,2	$E_{4.3},E_{4.6}$
	M	$[Pbcn,P42_12]$ (τ_2)	6	L_6	I,II	2,2	$T_{6.1},E_{6.2}$
		$[I\bar{4}2d,R\bar{3}]$			VI,IV	4,4	$E_{6.2},T_{6.2}$
$Pm3n$	Γ	$P4_222,P\bar{4}2c,P4_2/m,R\bar{3},P\bar{4}m2,R32$		. . .			
	R	$[Fmmm,I4_122](\tau_3+\bar{\tau}_3,\tau_4+\bar{\tau}_4)$	4	48.1	I,II	2,2	$E_{4.3},E_{4.6}$
	X	$[Pmma,P4_{1,3}22]$ (τ_3,τ_4)	6	L_9	I,II	2,2	$(E_{6.1}-A_{6.1}),E_{6.2}$
		$P\bar{4}2_1c$			VI	4	$E_{6.2}$
	M	$P4_2/ncm(\tau_3,\tau_4)$	3	O	I	2	$E_{3.1}$
		$[P4_2/mnm(\tau_7,\tau_8)P4_2/mcm(\tau_9,\tau_{10})$	3	O_h	I	2	$E_{3.1}$
		$[Pnna,Cmma]$ (τ_6)	6	L_7	I,II	2,2	$T_{6.1}(E_{6.1}-A_{6.2})$
		$[I4_1/acd,I4_1/acd,R32]$			VI,VII,IV	4,4,4	$E_{6.1},E_{6.1},T_{6.2}$
$Pn3m$	Γ	$P4_222,P\bar{4}2m,P4_2/n,R\bar{3},P\bar{4}n2,R32$		. . .			
	R	$[I4_1/amd,I4_1/acd](\tau_3,\tau_8)$	2	C_{6v}	I,II	2,2	$E_{2.1},E_{2.1}$
	X	$[Cmca,P4_{1,3}22]$ (τ_3,τ_4)	6	L_4	I,II	2,2	
		$[P\bar{4}2_1m,R\bar{3}c,R\bar{3}c]$			VI,III,IV	4,8,8	$E_{6.2},T_{6.1},T_{6.1}$
	M	$[Pbcm,P4_22_12]$ (τ_4)	6	L_6	I,II	2,2	$T_{6.1},E_{6.2}$
		$[I\bar{4}m2,R\bar{3}]$			VI,IV	4,4	$E_{6.2},T_{6.2}$
$Fm3m$	Γ	$I422,I\bar{4}2m,I4/m,R\bar{3},I\bar{4}m2,R32$		. . .			
	X	$P4/mnc(\tau_2)P4_2/mnm(\tau_3)$	3	O	I	2	$E_{3.1}$
		$P4/nnc(\tau_6)P4/nmm(\tau_7)P4_2/nmc(\tau_8)P4_2/nnm(\tau_9)$	3	O_h	I	2	$E_{3.1}$
		$[Pmmm,Cmcm]$ (τ_{10})	6	L_7	I,II	2,2	$T_{6.1},(E_{6.1}-A_{6.2})$
		$[P4/nmm,P4_2/mnm,R32]$			VI,VII,IV	4,4,4	$E_{6.1},E_{6.1},T_{6.2}$
	L	$R\bar{3}m(\tau_1,\tau_4)R\bar{3}c(\tau_2,\tau_5)$	4	109.01	I	2	$T_{4.1}$
		$[B2/b,B2/m](\tau_3)[B2/m,B2/b](\tau_6)$	8	M_2	I,II	2,2	$(T_{8.1}-E_{8.1}),(T_{8.1}-E_{8.1})$
		$[I4/mcm,I4/mmm](\tau_3)[I4/mmm,I4/mcm](\tau_6)$			IV,V	8,8	$E_{8.1},E_{8.1}$
		$Cmma(\tau_3)Cmmm(\tau_6)$			III	4	$T_{8.2}$
	W	$[I4/mmm,I4_1/amd](\tau_1,\tau_4)[I4/mcm,I4_1/acd](\tau_2,\tau_3)$	6	L_1	I,II	4,4	$E_{6.1},E_{6.1}$

TABLE IX. *(Continued)*

HS group	BZ point	Low-symmetry phases	OP dim	(a)	(b)	(c)	(d)
$Fm3c$	Γ	$I422,I\bar{4}2m,I4/m,R\bar{3},I\bar{4}m2,R32$		. . .			
	X	$P4/mbm(\tau_1)P4_2/mbc(\tau_4)$	3	O	I	2	$E_{3.1}$
		$P4/ncc(\tau_6)P4/nbm(\tau_7)P4_2/nbc(\tau_8)P4_2/ncm(\tau_9)$	3	O_h	I	2	$E_{3.1}$
		$[Pbcm,Cmcm]$ (τ_{10})	6	L_7	I,II	2,2	$T_{6.1},(E_{6.1}-A_{6.2})$
		$[P4_2/nmc,P4/mnc,R32]$			VI,VII,IV	4,4,4	$E_{6.1},E_{6.1},T_{6.2}$
$Fd3m$	Γ	$I4_122,I\bar{4}2m,I4_1/a,R\bar{3},I\bar{4}m2,R32$		. . .			
	X	$[Pnma,P4_32_12]$ (τ_4)		L_6	I,II	2,2	$T_{6.1},E_{6.2}$
		$[P\bar{4}2_1m,R\bar{3}]$			VI,IV	4,4	$E_{6.2},T_{6.2}$
	L	$R\bar{3}m(\tau_1,\tau_4)(R\bar{3}c(\tau_2,\tau_5)$	4	115.01	I	2	$T_{4.1}$
		$[B2/b,B2/m](\tau_3)[B2/m,B2/b](\tau_6)$	8	M_1	I,II	2,2	$(T_{8.1}-E_{8.1})$, $(T_{8.1}-E_{8.1})$
		$[I\bar{4}c2,I\bar{4}m2](\tau_3)[I\bar{4}m2,I\bar{4}c2](\tau_6)$			IV,V	8.8	$(E_{8.1}-A_{8.1})$, $(E_{8.1}-A_{8.1})$
		$Cmca(\tau_3)Cmcm(\tau_6)$			III	4	$T_{8.2}$
$Fd3c$	Γ	$I4_122,I\bar{4}2m,I4_1/a,R\bar{3},I\bar{4}c2,R32$		. . .			
	X	$[Pnma,P4_{1,3}22]$ (τ_4)	6	L_6	I,II	2,2	$T_{6.1},E_{6.2}$
		$[P\bar{4}2_1c,R\bar{3}]$			VI,IV	4,4	$E_{6.2},T_{6.2}$
$Im3m$	Γ	$I422,I\bar{4}2m,I4/m,R\bar{3},I\bar{4}m2,R32$		. . .			
	H	$[P4/mmm,P4_2/mmc](\tau_3)[P4/nnc,P4_2/nnm](\tau_8)$	2	C_{6v}	I,II	2,2	$E_{2.1},E_{2.1}$
	N	$Cmca,P4/mbm,I4_1/amd(\tau_3)Cmca,P4_2/ncm,I4/mcm(\tau_4)$	6	L_6	I,II,VI	2,4,8	$T_{6.1},E_{6.1},E_{6.1}$
		$R\bar{3}c,R\bar{3}(\tau_3)R\bar{3}m,R\bar{3}(\tau_4)$			III,IV	8,8	$T_{6.1},T_{6.2}$
		$Ccca,P4/nbm(\tau_5)Cmma,P4_2/mnm(\tau_6)$	6	L_4	I,II	2,2	$T_{6.1},E_{6.1}$
		$Cmcm,P4_2/mcm(\tau_7)Cmcm,P4/nmm(\tau_8)$			I,II	2,2	$T_{6.1},E_{6.1}$
		$I4_1/acd(\tau_5,\tau_8)I4/mmm(\tau_6)I4/mmc(\tau_7)$			VI	8	$E_{6.1}$
		$R\bar{3}m(\tau_6,\tau_8)R\bar{3}c(\tau_5,\tau_7)$			III	8	$T_{6.1}$
		$R32(\tau_5,\tau_6)$			IV	8	$(T_{6.1}-A_{6.3})$
	P	$[I422,I4_122,I4/mmm]$ $(\tau_3+\bar{\tau}_3)$	4	74.1	I,II,III	4,4,4	$E_{4.1},E_{4.1},E_{4.2}$
		$[I4/mmm,I4_1/amd,I4_1/amd]$			IV,V,VI	4,4,4	$E_{4.2},E_{4.2},E_{4.2}$
$Ia3d$	Γ	$I4_122,I\bar{4}2d,I4_1/a,R\bar{3},I\bar{4}c2,R32$		. . .			
	H	$Pbca,P4_{1,3}22(\tau_3+\bar{\tau}_3,\tau_4+\bar{\tau}_4)$	4	48.1	I,II	2,2	$E_{4.3},E_{4.6}$

exceptions for the sake of a more compact presentation, the order is that of the international tables of x-ray crystallography.[44] Space groups have been specified by their international symbol corresponding to the standard setting of axes.[44]

Column 2 lists, for each HS group, the relevant points of the first Brillouin zone. Except for the simple cubic BZ, there is no universally used notation for these points. The adopted one refers to the space-group-representation tables of Zak *et al.*[45] The components of the $\vec{k}$ vector represented by each of the former points as well as the number of arms in the corresponding star are available in TTI and TTII. For each space group we have only reproduced the BZ points associated to active IR's (see Sec. II) which are related to transitions of the purely ferroelastic type. The results of the selection of active IR's were presented formerly in TTI and TTII for the BZ-boundary points and in Ref. 28 for the BZ center (Γ point).

Column 3 lists the ferroelastic LS space groups identified by their standard international symbol. The relative orientation of the LS and HS symmetry elements has only been specified when the knowledge of the ferroelastic species relative to the transition was not entirely determined by the LS group. Thus we do not distinguish in the tables the point-symmetry changes $mmm \rightarrow 2^z/m$ and $mmm \rightarrow 2^y/m$ as both correspond to the same species and to the same spontaneous-strain component, within a permutation of the corrdinates. By contrast, the symmetry changes $4/mmm \rightarrow 2^z/m$ and $4/mmm \rightarrow 2^x/m$ are physically distinct,[11] and their respective occurrence has been shown in the tables. The IR inducing a LS phase is indicated by the symbol τ_i of the small representation referred to Zak's table for the HS space group. Whenever identical LS phases arise from different IR's at the same BZ point, the symbols for the various small representations are grouped together between parentheses following the symbol of the LS group. On the other hand, each τ_i corresponds, in general, to several LS phases with distinct symmetries. These phases are either grouped between square brackets on the same line of the table, or listed on consecutive lines.

Column 4 states the dimension of each relevant IR. This dimension is equal to the number of components of the transition's order parameter.

Column 5 contains the symbols for the images of the IR's. These symbols refer to Table V for OP dimensions in the range 1–3, to Fig. 1 for an OP dimension of 4, and to Fig. 2 for OP dimensions equal to 6 and 8. As stressed in Sec. III, one then has access through Tables II and III (and Ref. 37 for lower-dimensional images) to the form of the OP expansions.

Column 6 of Tables VI–IX specifies by a symbol (referred to Tables II, III, and V) the direction in ϵ associated to each ferroelastic phase. In addition, column 7 indicates the change in the number of atoms in the crystal's unit cell which accompanies the lowering of symmetry. Whenever several indications are contained in these columns, they are placed in the same order as the corresponding phases located between brackets.

Column 8 is relative to the construction of the term representing the coupling between the OP and the spontaneous strain (or higher-rank-tensorial components when the considered ferroelastic species is not a "full" one). The symbol contained in this column refers to Table IV and specifies a set of homogeneous polynomials ψ_j (see Sec. III) spanning an IR of the HS point group and associated to the relevant ferroelastic species. Whenever the latter species involves two distinct IR's, the corresponding symbols for the two sets of ψ_j functions are grouped between parentheses.

To illustrate by a simple example the use of the various tables, let us consider the PFT transitions which arise from the *Fmm*2 space group. As shown by Table VI, such transitions exist at the Γ and R points of the BZ.

The transition at the Γ point corresponds to the symmetry change $Fmm2 \rightarrow B2$ (column 3) without change of the number of atoms in the unit cell (column 7). It is induced by the one-dimensional IR (τ_3) (columns 3 and 4), and it can be classifed as a proper ferroelastic transition (column 8). Thus, its OP can be taken as the spontaneous-strain component spanning τ_3. Referring to the species $mm2 \rightarrow 2$ in Table I, we find that this component is the pure shear x_6. As explained in Sec. III, the Landau free energy for this transition can therefore be written

$$F=(C_{66}/2)x_6^2+(C'/4)x_6^4 \ . \tag{3}$$

The space-group change at the R point is also $Fmm2 \rightarrow B2$. It corresponds to the same ferroelastic species $mm2 \rightarrow 2$ and to the same spontaneous strain x_6 but, as shown by column 7, it is accompanied by a fourfold expansion of the unit cell. By contrast to the former one, this PFT transition is of the improper type.

It appears from Table VI (columns 4 and 5) that the OP is four dimensional and that its symmetry properties are described by the image denoted 56.1.

This image gives rise to an OP expansion labeled f_5 (Fig. 1) whose expression is (Table II)

$$\begin{aligned} f_5=&\tfrac{1}{2}\alpha\left(\sum_{1,4}\eta_i^2\right)+\tfrac{1}{4}\beta_1\left(\sum_{1,4}\eta_i^4\right)+\tfrac{1}{2}\beta_2(\eta_1^2\eta_2^2+\eta_3^2\eta_4^2)\\ &+\tfrac{1}{2}\beta_3(\eta_1^2\eta_3^2+\eta_2^2\eta_4^2)+\tfrac{1}{2}\beta_4(\eta_1^2\eta_4^2+\eta_2^2\eta_3^2)\\ &+\beta_5\eta_1\eta_2\eta_3\eta_4 \ . \end{aligned} \tag{4}$$

Such an expansion is compatible (Table II) with six distinct LS phases depending on the relative values of the β_i coefficients.

When the HS group is *Fmm*2, the only LS phase associated to ferroelasticity is the one labeled IV and corresponding to the [1001] direction in the representation space ϵ. The function labeled $A_{4.1}$ (column 8 of Table VI) of the OP components, transforms like the spontaneous strain x_6. Its expression is supplied by Table IV within a permutation of the OP components (among the various possible expressions the one to be retained is nonzero for the [1001] direction in ϵ). Accordingly, the term representing the coupling between x_6 and (η_i) components can be written (Sec. III)

$$\begin{aligned} F_3(\eta_i,x_6,\delta)&=\delta x_6 A_{4.1}\\ &=\delta x_6(\eta_1^2+\eta_4^2-\eta_2^2-\eta_3^2) \ . \end{aligned} \tag{5}$$

On the other hand, the truncated elastic energy of the crystal, limited to the x_6 component is[43]

$$F_2=(C_{66}/2)x_6^2 \ . \tag{6}$$

The required LFE associated to the considered transition is the sum of Eqs. (4)–(6).

The crystallographic information contained in the tables is not complete, in that it does not state explicitly the primitive translations of the LS phases. However, possible translational modifications accompanying continuous phase transitions have been worked out formerly by Lifshitz[46] and in a more complete way by Naish *et al.*[17] By reporting to these tables on the basis of the indications of Tables VI–IX, one is able to obtain unambiguously the missing data. Thus, in the case of the considered transition the k vector relative to the R point is[3,45] $\vec{k}=[\frac{1}{2},\frac{1}{2},\frac{1}{2}]$. For this $\vec{k}$ vector Naish's tables[47] indicate a single translational change compatible with the fourfold unit-cell expansion of the crystal.

For many of the 188 considered space groups, the situation is more complex than in the preceding example. Thus, the *Fm*3*m* space group (Table IX) is likely to give rise to 39 ferroelastic phases corresponding to 20 different IR's with dimensions ranging from 2 to 8. However, working out the characteristics of each transition can be achieved, using the tables, indentically as above.

The crystallographic part of the results contained in the tables could partly be checked by comparison to previous group-theoretical work available for the HS space groups $Pm3m$,[7,48] $Pm3n$,[49] $Fd3m$,[50] and other simpler groups. A more extensive comparison could be made to the unpublished work of Syromiatnikov,[51] where subgroups of the 230 space groups have been ordered according to the loss of translational symmetry related to each one of the $\vec{k}$ vectors permitted by the Lifshitz criterion. However, this author has based his crystallographic investigation on principles[52] which coincide with those of the Landau theory only when the small representation τ_i is one dimensional. In the other cases, which correspond to most of the transitions considered here, the symmetries indicated in his tables have no relevance to the Landau theory.

B. Discussion and comparison to the experimental data

We have listed in Tables X and XI materials representative of the main structural families undergoing purely ferroelastic transitions. Table X contains 17 examples of "proper" transitions, and Table XI 22 examples of "improper" ones. In most of the selected examples, reliable data are available on the space groups of the two phases, thus allowing a comparison to the results obtained in the present work.

The theoretical results of Tables VI–IX show that three groups of transitions can be distinguished on the basis of the characteristics of their order parameter and of the symmetry change. The first group contains the transitions arising from HS space groups of the monoclinic, orthorhombic, and tetragonal systems, the second one concerns the trigonal-hexagonal systems, and the third one the cubic system.

C. Monoclinic, orthorhombic, and tetragonal systems

Most of the PFT in these systems are predicted to comply with a uniform scheme.

Thus, with one exception (in the $4/m$ class), proper transitions should have a one-dimensional OP determining a subgroup of index 2 for the LS phase. Actual examples shown in Table X fit strictly into this scheme. For instance, the symmetry changes observed in NdP_5O_{14} (Ref. 13) (HS phase in the orthorhombic system) or in $DyVO_4$ (tetragonal system)[14] as well as those of five other families of substances, confirm the results listed in Tables VI–VII. All these transitions are observed to be continuous. As expected for a proper PFT,[31] a definite combination of elastic constants vanishes at the Curie point for several of these substances, namely, NdP_5O_{14}, $KH_3(SeO_3)_2$, TeO_2, $DyVO_4$, and $TbVO_4$. No elasticity

TABLE X. Materials possessing a proper ferroelastic transition.

Substance	T_c(K)	Order	Symmetry change		OP dimension	Table number	Reference
			HS	BZ			
NdP_5O_{14}	420	2	$Pmna$	$P2_1/b$	1	VI	13
$KH_3(SeO_3)_2$	212	2	$Pbcn$	$P2_1/b$	1	VI	14
$BiVO_4$	528	2	$I4_1/a$	$B2/b$	1	VII	18
$LaNbO_4$	770	2	$I4_1/a$	$B2/b$	1	VII	80
$LaNbThTiO_8$	950	2	$I4_1/a$	$B2/b$	1	VII	81
TeO_2	8 kbar	2	$P4_12_12$	$P2_12_12_1$	1	VII	82
$DyVO_4$	14	2	$I4_1/amd$	$Imma$	1	VII	24
$TbVO_4$	33	2	$I4_1/amd$	$Fddd$	1	VII	24
NaN_3	293	2	$R\bar{3}m$	$B2/m$	2[a]	···	62
s-triazine	210	1	$R\bar{3}c$	$B2/b$	2[a]	···	61
$K_2Mn_2(SO_4)_3$	200	1	$P2_13$	$P2_12_12_1$	2[a]	···	71
$RbAg_4I_5$	208	2	$P4_132$	$R32$	3[a]	···	83
V_3Si	21	2	$Pm3n$	$P4_2/mmc$	2[a]	···	21
KCN	170	1	$Fm3m$	$Immm$	2[a]	···	69
InTl	320	1	$Fm3m$	$I4/mmm$	2[a]	···	70
KNO_2	295	1	$Fm3m$	$R\bar{3}m$	3[a]	···	72
$NiCr_2O_4$	274	1	$Fd3m$	$I4_1/amd$	2[a]	···	24

[a] Order parameters not complying with Landau's (symmetric cube) condition.

TABLE XI. Materials possessing an improper ferroelastic transition.

Substance	T_c(K)	Order	Symmetry change		Unit cell	OP		Table number	References
			HS	LS	X	BZ point	dimens.		
P-terphenyl	178	2	$P2_1/b$	$P\bar{1}$	2	C	2	VI	19
$C_4O_4H_2$	470	1	$I4/m$	$P2_1/m$	2	Z	2	VII	20
ADP	148	1	$I\bar{4}2d$	$C222_1$	2	Z	2	VII	12
$RbFeF_4$	570	2	$P4/mmm$	$Pmma$	2	Z	2	VII	84
VO_2	343	1	$P4_2/mnm$	$P2_1^x/b$	2	R	4	VII	3
Hg_2Cl_2	185	2	$I4/mmm$	$Cmcm$	2	X	2	VII	15
$(CH_3NH_3)_2CdCl_4$	484	2	$I4/mmm$	$Cmca$	2	X	2	VII	85
$Ag_2H_3IO_6$	241	2	$R\bar{3}$	$P\bar{1}$	2	M	3	VIII	57
$Pb_3(PO_4)_2$	453	1	$R\bar{3}m$	$B2/b$	2	L	3	VIII	58
Sb_5O_7I	481	1	$P6_3/m$	$P2_1/b$	2	M	3	VIII	55
K_2SeO_4	745	. . .	$P6_3/mmc$	$Pnma$	2	M	3	VIII	56
$(NH_4)_2SO_4$	. . .	. . .	$\left\{\begin{array}{l}P6_3/mmc\\P6_3/mcm\end{array}\right.$	$Pnma$	2	M	3	VIII	60
$CdSnAs_2$	840	1	$F\bar{4}3m$	$I\bar{4}2d$	4	W	6	IX	67
$ZnSnAs_2$	920	1	$F\bar{4}3m$	$I\bar{4}$	4	W	a	. . .	67
Ag_2HgI_4	323	1	$F\bar{4}3m$	$I\bar{4}$	4	W	a	. . .	73
$SrTiO_3$	196	2	$Pm3m$	$I4/mcm$	2	R	3	IX	63
$NdAlO_3$	1640	2	$Pm3m$	$R\bar{3}c$	2	R	3	IX	64
NH_4Br	235	2	$Pm3m$	$P4/nmm$	2	M	3	IX	65
CuAu	653	1	$Fm3m$	$P4/mmm$	2	X	3	. . .	66
N_3AlF_6	830	. . .	$Fm3m$	$P2_1/b$	2	X	a	. . .	74
$SmAlO_3$	. . .	. . .	$Pm3m$	$Pnma$	. . .	. . .	a	. . .	75
$Cs_2NaLnCl_6$	. . .	. . .	$Fm3m$	$I4/m$	1		3	IX	68

[a] Reducible order parameter.

measurements are available yet for $BiVO_4$, $LaNbO_4$, and $LaNbThTiO_8$, but due to their compliance with the same symmetry scheme, they should display the same characteristic elastic softening.

On the other hand, for the three considered crystal systems, a standard type of improper PFT is expected to occur, associated to a two-dimensional OP whose image is either C_4 or C_{4v}. The symmetry change, leading to a subgroup of index 4, consists in a twofold decrease of the point symmetry (e.g., $2/m \rightarrow \bar{1}$, $mmm \rightarrow 2/m$, $422 \rightarrow 222$, $4/mmm \rightarrow mmm$), and in a doubling of the number of atoms in the primitive unit cell. The ferroelastic strain is a quadratic function of the OP. This simple pattern is the one previously studied in detail for the ferroelectric-ferroelastic transition in gadolinium molybdate,[4] and it is therefore expected to remain valid for a large number of compounds. Consistently, six out of seven examples available for the considered crystal systems (Table XI) have symmetry changes complying with this description. For all these materials, the salient features of the physical behavior should resemble those of gadolinium molybdate. In particular, elastic constants should undergo a discontinuous downward jump at the onset of the LS phase (even for a perfectly continuous transition[31]). The only data which can be compared to this prediction are the ones for Hg_2Cl_2,[53] and $C_4O_4H_2$,[54] and they are in clear agreement with it.

Other types of more complex schemes are possible in a few orthorhombic and tetragonal space groups. They all correspond to four-dimensional OP.

For instance, orthorhombic space groups having an F-centered lattice give rise to a four-dimensional OP at the R point $(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})$ of the BZ, since the star k^* at this point has four arms. Such an OP induces unit-cell multiplications by factors of 2, 4, or 8, and to the unusual point-symmetry change $mmm \rightarrow \bar{1}$, which would be impossible at the BZ center because no IR of the mmm point group is related to it. Its possibility in a continuous transition at the preceding BZ-boundary point is due to the simultaneous coupling of the OP to several IR's of mmm. The triclinic phase can be considered as the result of the simultaneous onset of several, differently oriented, monoclinic phases (e.g., $2^x/m$, and $2^y/m$).

A similar scheme is found for the tetragonal space groups with a body-centered lattice, at the N point of the BZ boundary.

No examples for these types of transitions seem to have been detected yet in real physical systems.

By contrast, the ferroelastic, metal-insulator transition in VO_2,[3] (Table XI), though strongly discontinuous, provides a good illustration of an exceptional pattern displayed by only two space groups of the tetragonal system, i.e., $P4/mnc$ (D_{4h}^{6}) and $P4_2/mnm$ (D_{4h}^{14}) at the R point $(\frac{1}{2},0,\frac{1}{2})$ of the BZ. The symmetry properties of the corresponding four-dimensional OP determine, in particular, the possibility of transitions towards both the $2^x/m$ and $2^z/m$ point groups which have, respectively, been observed in pure, and chromium-substituted VO_2.

It is worth noting that for the three considered systems, about 1000 different types of continuous symmetry changes are predicted to be possible accompanied by a lowering of both the point and the translational symmetries (improper ferroic transitions[10]): among these, over 800 are ferroelastic ones.

D. Trigonal and hexagonal systems

As shown by Table VIII, in these systems, PFT are mainly induced by three-dimensional order parameters at the M point $(\frac{1}{2},0,0)$ for all the investigated space groups, and at the L point $(\frac{1}{2},0,\frac{1}{2})$ for all symmorphic space groups. The ferroelastic phase corresponds to the [100] direction in the representation space (Table V). It is associated with a threefold lowering of point symmetry and to a double unit cell with respect to the HS phase. At the M point, the double periodicity is located in the plane perpendicular to the ternary or senary axis. At the L point it occurs along a skew orientation.

The symmetry changes predicted for the M point are in good agreement with the experimental data relative to the transitions in Sb_5O_7I,[55] K_2SeO_4,[56] and $Ag_2H_3IO_6$.[57] Likewise in lead orthophosphate $Pb_3(PO_4)_2$, both the crystallographic modifications and the occurrence of a triply degenerate soft mode at the L point[58] are observed to comply with the theoretical results.[59]

A similar "latent" transition has been assumed to exist in $(NH_4)_2SO_4$ in order to explain the ferroelastic behavior of the room-temperature orthorhombic $Pnma$ phase.[60] The speculative HS phase has been assigned the $P6_3/mmc$ space group on the basis of a group-subgroup relationship between phases and of the relative orientation of the ferroelastic domains. Inspection of Table VIII shows that this is not the only possible group, and that $P6_3/mcm$ could equally well fulfill the symmetry requirements. In either case the order parameter of the transition would correspond to the M point of the BZ boundary.

Thus, the available examples of improper ferroelastics agree satisfactorily with the theoretical scheme. However, no illustration seems to exist for another type of improper PFT arising from a two-dimensional OP at the A point $(0,0,\frac{1}{2})$ of the BZ boundary. Its symmetry properties are represented by the images C_6 or C_{6v} (Table V). They therefore differ from the two-dimensional OP encountered in the monoclinic, orthorhombic, and tetragonal systems. The symmetry change induced would correspond to a threefold decrease of the point symmetry (e.g, $\bar{3}m \rightarrow 2/m$; $6/mmm \rightarrow mmm$) and to a doubling of the periodicity along the ternary or senary axis.

On the other hand, as shown by Table X, at least two examples of proper PFT are known, namely, s triazine[61] $C_3H_3N_3$, and sodium azide[62] NaN_3. This situation contrasts with the fact that no continuous transitions are predicted to be possible at the Γ point of the trigonal and hexagonal space groups (with the exception of the $6/m$ and $6/mmm$ classes). This is due to the noncompliance of the relevant two-dimensional IR's with the Landau criterion (symmetric cube). Consequently the induced transitions should be discontinuous. Experimental results[61] show that the transition in s triazine is indeed of first order, though slightly so. As for NaN_3 its transition is claimed to be continuous, within experimental accuracy.[62]

It is therefore striking to note that the transitions in these two materials, which do not fulfill Landau's criterion, display discontinuities of similar magnitudes as the transition in lead phosphate which complies with this criterion.

E. Cubic system

Unlike the other crystal systems, the cubic one displays a large variety of situations with respect to the OP dimensions, the lowering of symmetry and the coupling scheme between the OP and the macroscopic tensors (Table IX).

Let us examine first the PFT which are accompanied by a decrease of the translational symmetry. Two cases can be distinguished among them.

The first one corresponds to the same standard type of three-dimensional OP which are encountered in the trigonal system. The PFT involve a lowering of point symmetry by a factor of 3 (e.g., $m3m \rightarrow 4/mmm$) or 4 (e.g., $m3m \rightarrow \bar{3}m$) together with a doubling of the primitive unit cell. They can arise at the R point $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, the X point $(0,0,\frac{1}{2})$, and the M-point of the simple cubic BZ, and also at the X point $(\frac{1}{2},\frac{1}{2},0)$ of the fcc space groups (Table IX).

Several continuous transitions are found to comply with this description. This is, for instance the case of the ferroelastic perovskites isomorphous of $SrTiO_3$,[63] and $NdAlO_3$,[64] and of the order-disorder transition in ammonium bromide NH_4Br.[65] A related pattern also occurs in the metallic alloys of the CuAu I type.[66] In the latter materials the point, and translational symmetry change are consistent with a three-dimensional

OP at the X point of the $Fm3m$ space group. However, this OP does not fulfill the Landau criterion. In agreement with it, the transitions are observed to be strongly discontinuous, and to display a large thermal hysteresis.

Symmetry-change patterns without a counterpart in lower-symmetry systems are mainly related six- and eight-dimensional order parameters.

Six-dimensional IR's are determined in a variety of ways. At the X and M points (sc lattice) and at the X point (fcc lattice) already mentioned above, they correspond to a three-arm star and a two-dimensional small representation. At the N point $(\frac{1}{2},0,0)$ of the bcc Brillouin zone and at the W point $(\frac{3}{4},\frac{1}{2},\frac{1}{4})$ of the fcc one, they result from a six-arm star and a one-dimensional small representation. No uniform scheme of symmetry changes is found for these representations since the OP symmetries are related to 10 distinct images (Fig. 2). Thus point symmetry changes from $m3m$ towards seven different classes of the orthorhombic, tetragonal, and rhombohedral systems are predicted to be possible, as well as unit-cell multiplications by factors of 2, 4, and 8.

On the other hand, eight-dimensional IR's occur at the L point of the fcc lattice. They induce the steepest decrease in symmetry which is obtained for all the investigated transitions. Thus the index of the LS space group with respect to the HS one can be as high as 48. For instance, a continuous transition is predicted from $Fd3m$ to $I\bar{4}m2$, with an eightfold expansion of the unit cell. These types of OP are also the only ones compatible with certain ferroelastic species (e.g., $m3m \to 2^{xy}/m$, or $m3 \to \bar{1}$) which involve a large decrease in point symmetry.

Few examples have been found, up to now, of structural transitions possessing such high-dimensional order parameters. In the case of pure ferroelastics, a representative class of substances is provided by the ternary semiconductors undergoing a reversible transition from the chalcopyrite structure ($I\bar{4}2d$) to the zinc blend one ($F\bar{4}3m$). These transitions have previously been pointed out by Jerphagnon[67] to be related to improper PFT. The number of atoms in the primitive unit cell is multiplied by 4, and Table XI allows us to identify unambiguously the OP as a six-dimensional one at the W point of the BZ. $CdSnAs_2$ and $ZnGeAs_2$ are two examples of these substances with transitions, respectively, occurring at 840 K and 1080 K.[67]

Let us consider now the transitions which preserve the number of atoms in the crystal's unit cell. A remarkable feature of the cubic system is that continuous equitranslational ferroelastic transitions are only possible if their order parameter is distinct from the components of a homogeneous strain. These unusual types of improper ferroelastics are associated to two- and three-dimensional OP having the symmetries either of a third-rank polar tensor (e.g., $m3 \to 222, 4\bar{3}m \to \bar{4}, m3m \to 422$) or of components of a fourth-rank polar tensor (e.g., $m3m \to 4/m$, $m3m \to \bar{3}$). The onset of the spontaneous strain of these ferroelastic species is due to the coupling of the strain components to quadratic polynomials of the former macroscopic quantities, whose form is specified in Tables IX and IV.

Possible examples of such improper PFT can be found among compounds with the formula $Cs_2NaLnCl_6$ (Ln:lanthanide) belonging to the family of elpasolites.[68] These have been conjectured to undergo the symmetry change $Fm3m \to I4/m$ with one formula per unit cell in both phases. As stressed above, the OP would correspond to the components of a fourth-rank tensor, namely, the three-dimensional set of elastic constants $(C_{24}-C_{34};C_{35}-C_{15};C_{16}-C_{26})$ (Table I).

By contrast, no continuous transition of the proper type is expected to occur because the corresponding OP do not comply with Landau's criterion.

As shown by Table X, a number of proper PFT have been observed in real crystals. Most of them possess a strong first order in agreement with the theoretical predictions. These are, for instance the transitions in KCN and NaCN,[69] those arising in several members of the spinel family,[24] as well as those observed in many martensitic transformations similar to the one in the indium thallium alloys.[70] Some compounds with the langbeinite structure[71] and potassium nitrite KNO_2 (Ref. 72) also belong to this class of transitions. A few examples, however, possess transitions which are almost continuous. In particular, V_3Si has been the subject of many accurate investigations which have assigned to its 21 K transition a continuous character.[21]

Finally, we can note that the experimental data contain examples of symmetry changes which do not comply with the most important feature of Landau's theory: they do not appear to be induced by a single IR of the HS phase.

Thus, the symmetry change in Ag_2HgI_4,[73] and $ZnSnAs_2$ (Ref. 67) ($F\bar{4}3m \to I\bar{4}$, with a fourfold unit-cell expansion) cannot be accounted for by the IR's considered in Table IX, though the translational change matches well the one predicted at the W point. The full symmetry change is probably associated to a reducible order parameter composed of a six-dimensional IR at the W point, and of three-dimensional one at the Γ point. Also, the transition in cryolithe N_3AlF_6 (Ref. 74) ($Fm3m \to P2_1/b$, with a double unit cell) involves several IR's, one of which corresponds to the X point of the BZ boundary. Other complex examples have been pointed out[48] to occur in the ferroelastic-antiferromagnetic perovskites such as $SmAlO_3$,[75] or $LaFeO_3$ (Ref. 76) (Table XI).

IV. CONCLUSION

In this paper, a theoretical investigation has been carried out of the symmetry characteristics of purely ferroelastic transitions. We have established that, in the strict framework of Landau's theory of continuous transitions, this type of transition should constitute the largest part of the ferroic transitions encountered in crystals. By comparison, other categories of structural transitions previously examined in TTI and TTII (i.e., purely ferroelectric transitions, secondary ferroics, etc.) correspond to marginal cases. In particular, while improper ferroelectrics were noted to be an exception, on theoretical grounds improper ferroelastics appear to be the rule.

In the theoretical procedure adopted to handle this systematic application of Landau's theory, we have stressed the similarity which exists between transitions arising from different high-symmetry space groups with respect to the symmetry properties of the order parameter, and to the pattern of the possible low-symmetry phases. As already pointed out by previous authors,[29,37] we have shown that this similarity relies on the occurrence of an identical "image" for the various order parameters considered. To be able to deal with the case of order parameters of dimensions greater than 3, mostly arising in the cubic system, we have established for the first time the form of the corresponding images, and their mutual relationship.

As a result of identifying the different images, we could show that the symmetry and thermodynamical aspects of Landau's theory of continuous transitions is contained in the properties of 49 images of dimensions ranging from 1 to 8, and giving rise to, at most, 49 types of free-energy expansions.

The enumeration of all possible ferroelastic transitions of the continuous type has been presented in tables. These tables allow a determination of the crystallographic modifications (point and translational symmetry) taking place at each transition, a deduction of the dimension and symmetry properties of the order parameter associated to it, as well as of the free-energy expansion.

A comparison of these theoretical results to the experimental data available for ferroelastic transitions in real substances has been performed. It has shown that the experimental results can be classified into three groups.

The first and largest group is constituted by the continuous or discontinuous transitions which comply in all their symmetry and thermodynamical aspects with the results contained in the tables. Among the 39 examples of materials selected for the reliability of the data available for them, 25 were found to belong to this group. For each such material, starting from the knowledge of the space-group change, the usefulness of the tables consists in the possibility of deducing, by simple inspection, the information which is necessary to elaborate a phenomenological theory of the considered transition. Belong to this group, all the transitions observed in lower-symmetry systems (monoclinic, orthorhombic, tetragonal) as well as most of the transitions in any system which are accompanied by a multiplication of the unit cell of the crystal. We can note that the latter "improper" ferroelastic transitions outnumber the examples of ferroelastics which preserve the crystal's periodicity. This situation contrasts with the case of improper ferroelectrics for whom examples were scarce[10] and difficult to understand on the basis of Landau's theory.

A second group of transitions corresponds to equitranslational symmetry changes which fail to comply with Landau's "symmetric-cube" criterion. These transitions have a high-symmetry phase belonging to the trigonal or cubic system. Their characteristics cannot be found in the present tables (I–XI). However, their order-parameter and free-energy expansion are available in the tables of Janovec *et al.*,[28] which contain the characteristics of all the cell-preserving transitions.

Finally a few cases remain of materials in which a first-order transitions appears to be induced by a reducible order parameter. Such cases could be easily detected by inspection of the tables since, for them, either the point-symmetry change or the translational symmetry one did not fit into the listed results. For each such example, it would be necessary to perform a particular group-theoretical analysis of its symmetry characteristics in order to interpretate the physical pecularities of its transition. In some ferroelectric materials analyses along these lines have recently been carried out to explain intricate symmetry changes, namely, in the boracites,[77] Rochelle salt,[78] and benzil.[79]

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APPENDIX

In this Appendix, we show that, if the possibility of a line of continuous transitions between G_0 and G has been established on the basis of the order-parameter expansion, this possibility will be preserved when the coupling with the strain is taken into account. As stressed in Sec. III, the OP expansion can be written

$$F_1(\alpha,\eta_i,\beta_k)=(\alpha/2)\left[\sum_i \eta_i^2\right]+\sum\nolimits_k \beta_k f_k(\eta_i)\ , \tag{7}$$

where the f_k are invariant polynomials of degree $\geqslant 4$. A line of continuous transitions between G_0 and G is assumed to exist for $\beta_k^1 < \beta_k < \beta_k^2$ (strict inequality). Let us first introduce the coupling with a single strain component x. The Landau free energy will be expressed as

$$F=F_1+(C/2)x^2+\delta x\psi(\eta_i)\ . \tag{8}$$

For a mechanically free crystal, the strain can be eliminated from Eq. (8) through the condition $\partial F/\partial x=0$ resulting in

$$F=F_1-(\delta^2/2C)\psi^2(\eta_i)\ . \tag{9}$$

Continuous transitions are determined by the absolute minima of F. Like F and F_1, the homogeneous polynomial $\psi^2(\eta_i)$ is invariant by G_0. Its degree is $2p \geqslant 4$ (ψ being of degree $\geqslant 2$ since x and η_i implicitly have different symmetries). If $2p$ is greater than the highest degree in F_1, ψ^2 will obviously have no influence on the stability of the LS phases just below the transition point. A line of continuous transition will exist for unmodified ranges of the β_k coefficients, no condition being imposed to δ.

In the other case, ψ^2 can be expressed as a linear combination of the f_k (with some of the coefficients possibly zero)

$$\psi^2/2C=\sum_k \gamma_k f_k\ . \tag{10}$$

Inserting Eq. (10) into Eq. (9) shows that F takes the same form as F_1 with the modified coefficients

$$\beta_k''=\beta_k-\delta^2\gamma_k\ . \tag{11}$$

Let δ_0^2 be a finite quantity smaller than the set of values $|(\beta_k^2-\beta_k^1)/\gamma_k|$, for $\gamma_k \neq 0$. If we impose the following conditions on the expansion coefficients:

$$\begin{aligned}
&|\delta| < |\delta_0|\ ,\\
&(\beta_k^1 < \beta_k < \beta_k^2)\ \text{ if } \gamma_k=0\ ;\\
&(\beta_k^1 < \beta_k < \beta_k^2+\delta_0^2\gamma_k)\ \text{ if } \gamma_k<0\ ;\\
&(\beta_k^1+\delta_0^2\gamma_k < \beta_k < \beta_k^2)\ \text{ if } \gamma_k>0\ .
\end{aligned} \tag{12}$$

It can easily be checked that we have $\beta_k^1 < \beta_k'' < \beta_k^2$ and that, consequently, a line of continuous transitions exists between G_0 and G.

The preceding proof would not hold for transitions which can only be continuous at a definite temperature and pressure (p_0,T_0). Such a transition point would correspond to a condition of the type

$$\beta_{k0}^1(p_0,T_0)=\beta_{k0}^2(p_0,T_0)\ . \tag{13}$$

As in general the occurrence of $\gamma_{k0} \neq 0$ cannot be discarded, we will have

$$\delta=\delta_0=0\ . \tag{14}$$

The three equations (13), (14), and $\alpha(p_0,T_0)=0$, cannot be satisfied simultaneously, thus resulting in a supression of the continuous character of the transition.

When several strain components x_l are involved in the coupling terms, the free energy takes the more general form

$$F=F_1+\tfrac{1}{2}\sum C_{lm}x_l x_m+\sum \delta_l x_l \psi_l(\eta_i)\ . \tag{15}$$

The occurrence of a line of continuous transitions can be straightforwardly established using the same arguments as in the case of a single strain component by eliminating the x_l through the set of conditions $\partial F/\partial x_l=0$, and puting, for instance, δ equal to the largest of the δ_l coefficients.

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