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Comment on symmetry changes in $A15$ structure

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I clarified discrepancies found between the applications to $A15$ structure of the chain criterion and the Landau theory of second-order phase transitions. I also present complete determination via the chain criterion of all allowed low-symmetry groups based on X- and R-point representations for $A15$ (O_h^3) structure.

I. INTRODUCTION

Symmetry conditions contained in the Landau theory of second-order phase transitions have been the subject of some controversy for several years.[1] In particular, the chain criterion (CC) was criticized recently.[2,3] This criterion was introduced by Jarić.[4] However, the proof of the equivalence of the CC and the necessary symmetry condition contained in the original Landau theory (LNC) was not given in Ref. 4.

The CC was applied to the study of structural phase transitions in $A15$ structure, driven by an X- or R-point order parameter.[5,6] However, recent claims, based on calculations for $A15$ structure, were made that CC is not equivalent to Landau's necessary condition (LNC).[2,3] A new criterion, was introduced which is claimed to be equivalent to LNC.[3] Contrary to these claims, recently I proved rigorously the equivalence of CC, LNC, and the "proposition."[7,8]

The purpose of this paper is to clarify apparent differences found in the applications of CC and LNC to $A15$ structure as well as to complete with the help of CC a group theoretical analysis of structural phase transition in $A15$ structure, driven by an X- or R-point order parameter.

II. ANALYSIS FOR $A15$ (O_h^3) STRUCTURE

Recent criticism[2,3] of the CC was based on a comparison of results for $A15$ structure obtained by CC and LNC. In light of the general proof of equivalence presented in Ref. 7, any disagreement between CC and LNC results must be clarified.

Differences between the results of Ref. 5 and those of Refs. 2 and 3 are of two kinds. First, Refs. 2 and 3 eliminate some of the subgroups which seem allowed in Ref. 5. Second, Refs. 2 and 3 add some new allowed subgroups. These discrepancies have the following reason. The CC can be applied to any collection of subgroups of the high-symmetry group (O_h^3). The subgroups *eliminated* in such a way are eliminated exactly. However, considering additional subgroups, which are not in the original collection, can produce some additional eliminations. Also, since new subgroups are now added to the analysis, some of them may be allowed as well. Therefore, in order to make a complete determination of allowed subgroups, all subgroups of a high-symmetry phase must be examined. Apparently, this was not transparent in the original formulations of CC[4,5]; more explicit formulation may be found in Ref. 7.

Tables I and II of Ref. 5 display the results obtained by an application of CC to the subgroups with the doubling of fundamental translations in one and two directions, respectively. However, application of CC to subgroups with doubling in two direction *relative* to subgroups with doubling in one direction was not employed. This application of CC further eliminates some of the allowed subgroups from Table II, Ref. 5.[9]

The reason for some additional discrepancies is that in Ref. 5 only the subgroups with the primitive translational subgroups were considered (doubling in one or two directions for X-point and doubling in three directions for R-point representations). Subgroups with other (including nonprimitive) conventional unit cells were not considered. References 2 and 3 eliminate incompleteness of Ref. 5. However, the results of Refs. 2 and 3 are obtained by the use of LNC[3] and the full minimization.[2] In addition, above mentioned results neither demonstrate completeness of the lists of allowed subgroups,[10] nor do they explicitly present associated Bravais lattices. Therefore, and in order to complete results of Ref. 5 as well as to illustrate equivalence of CC and LNC, I present below the results of complete application of CC to structural phase transitions in $A15$ structure, driven by an X- or R-point order parameter.

TABLE I. Conventional basis vectors for the translation subgroups of the allowed low-symmetry groups (see Tables II and III). For the nonprimitive subgroups, the equivalent translation vectors are also given. The vectors are given in terms of the original basis vectors. The translation subgroups are given up to a conjugation. See Figs. 1 and 2.

Irreducible representation	Translational subgroup	Basis: $\vec{e}_1;\vec{e}_2;\vec{e}_3$	Equivalent translations	Unit cell volume
	a	(2,0,0);(0,1,0);(0,0,1)	...	2
	b	(2,0,0);(0,2,0);(0,0,1)	...	4
$^*\vec{X}$	c	(2,0,0);(0,2,0);(0,0,2)	...	8
	$d\sim b$	$(0,0,\bar{1});(\bar{2},\bar{2},0);(\bar{2},2,0)$	(0,2,0)	8
	$e\sim c$	$(\bar{2},2,0);(0,0,2);(2,2,0)$	(0,2,0)	16
	a	(1,1,0);(1,0,1);(0,1,1)	...	2
	$b\sim a$	$(1,1,0);(\bar{1},1,0);(0,0,2)$	(0,1,1)	4
$^*\vec{R}$	$c\sim a$	(2,0,0);(1,1,0);(0,0,2)	(1,0,1)	4
	$d\sim a$	$(\bar{1},1,2);(\bar{1},1,0);(\bar{1},\bar{1},0)$	(1,0,1)	4
	$e\sim a$	(2,0,0);(0,2,0);(0,0,2)	{(1,1,0), (1,0,1), (0,1,1)}	8

A general form of characters for X- and R-point representations is

$$\chi=\chi_1(-)^{n_1}+\chi_2(-)^{n_2}+\chi_3(-)^{n_3} \tag{1}$$

and

$$\chi=\chi_1(-)^{n_1+n_2+n_3}, \tag{2}$$

respectively, where (n_1,n_2,n_3) is a pure translation in the original basis, and χ_i depend only on the rotational part of a symmetry operation. The forms Eqs. (1) and (2) impose on allowed subgroups to have translational subgroups among these given in Table I and Figs. 1 and 2. The results of complete application of CC to *A*15 structure are given in Tables II and III.

In Table II I show allowed low-symmetry groups arising from an X-point order parameter. I give here, for the first time, *all* of the allowed low-symmetry

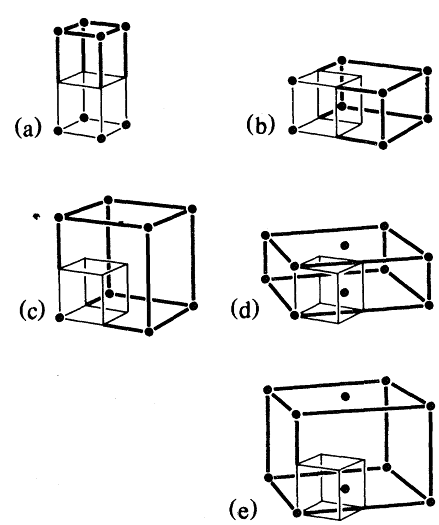

FIG. 1. Bravais lattices of the allowed low-symmetry groups based on X-point representations (full circles). The original Bravais lattice is also shown (light lines).

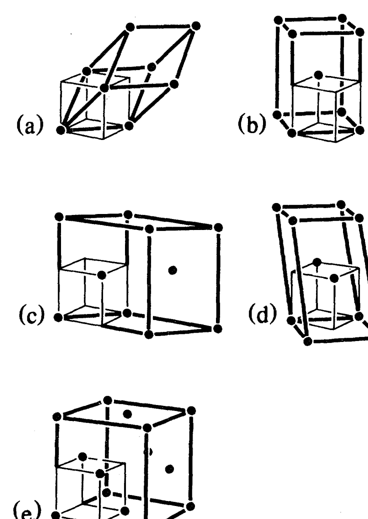

FIG. 2. Bravais lattices of the allowed low-symmetry groups based on R-point representations (full circles). The original Bravais lattice is also shown (light lines).

TABLE II. Phase transitions in O_h^3 based on X-point representations (see Ref. 5 for the notation).

Irreducible representation	Subduction frequency	Allowed subgroup (translational subgroup[a])
	6	$C_1^1(c)$
	5	$C_s^1(c)$
$^*\vec{X}(1)$	4	$C_{2v}^1(c)$, $C_s^1(b)$
	3	$D_{2h}^1(c)$, $C_{2v}^1(b)$, $C_2^3(e)$
	2	$D_{2d}^5(c)$, $D_{2h}^1(b)$, $C_{2v}^1(a)$, $C_{2v}^{16}(d)$, $C_3^4(c)$
	1	$T_h^1(c)$, $D_{4h}^9(b)$, $D_{2d}^5(a)$, $D_{2h}^1(a)$, $D_3^7(c)$
	6	$C_1^1(c)$
	5	$C_s^2(c)$
$^*\vec{X}(2)$	4	$C_{2v}^{10}(c)$, $C_s^2(b)$
	3	$D_{2h}^2(c)$, $C_{2v}^6(b)$, $C_2^3(e)$
	2	$D_{2d}^8(c)$, $D_{2h}^4(b)$, $C_{2v}^3(a)$, $C_{2v}^{17}(d)$, $C_3^4(c)$
	1	$T_h^2(c)$, $D_{4h}^{11}(b)$, $D_{2d}^6(a)$, $D_{2h}^3(a)$, $D_3^7(c)$
	6	$D_2^4(c)$
$^*\vec{X}(3)$	4	$D_2^3(b)$
and	3	$D_4^{4,8}(c)$, $D_{2h}^{15,16}(c)$
$^*\vec{X}(4)$	2	$T^4(c)$, $D_4^6(b)$, $D_{2d}^4(b)$, $D_{2h}^{9,11,13}(b)$, $D_2^2(a)$
	1	$O^{6,7}(c)$, $T_h^6(c)$, $D_{4h}^{13,15}(b)$, $D_4^{3,7}(a)$, $D_{2h}^5(a)$

[a]See Table I and Fig. 1.

groups, including nonprimitive ones as well as ones associated with the doubling of the unit cell in all three directions (the latter not being treated in Refs. 2 and 3).

Similarly, in Table III I show *all* allowed low-symmetry groups arising from an R-point order parameter. Note that in both Tables II and III new groups, not listed in Ref. 5, are given. In order to avoid confusion, all subgroups, for both X and R points, are listed here together with explicit forms of their translational subgroups which were not explicitly presented in Refs. 2 and 3.

TABLE III. Phase transitions in O_h^3 based on R-point representations (see Ref. 5 for the notation).

Irreducible representation	Subduction frequency	Allowed subgroup (translational subgroup[a])
$^*\vec{R}(1)$	2	$T^2(e)$
	1	$O^4(e)$, $T_h^3(e)$
$^*\vec{R}(2)$	4	$D_2^7(e)$
	2	$D_4^{10}(b)$, $D_{2h}^{23}(e)$
	6	$C_1^1(a)$
	4	$C_2^3(c)$
$^*\vec{R}(3)$	3	$C_2^3(d)$, $C_s^3(c)$, $C_i^1(a)$
	2	$S_4^2(b)$, $D_2^8(b)$, $D_2^7(e)$, $C_{2v}^{18}(e)$, $C_{2h}^3(c)$, $C_3^4(a)$
	1	$D_4^{10}(b)$, $D_{2d}^{11}(b)$, $D_{2h}^{23}(e)$, $D_3^7(a)$, $C_{3i}^2(a)$

[a]See Table I and Fig. 2.

III. CONCLUSIONS

I clarified the discrepancies in applications of CC and LNC to $A15$ structure. At the same time I completed with the help of CC the list of all allowed low-symmetry groups arising from X- or R-point order parameters. The results for X (doubling in one and two directions) and R points are identical with the corresponding ones of Ref. 3, however, the translational subgroups are given here explicitly. This is illustrative of the result that the CC is equivalent to LNC, which I proved rigorously elsewhere.[7] With respect to the experimental data, the conclusions of Ref. 5 remain essentially valid.

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[1]See, for example, A. P. Cracknell, J. Lorenc, and J. A. Przystawa, J. Phys. C 9, 1731 (1976).

[2]J.Lorenc, J. Przystawa, and A. P. Cracknell, J. Phys. C 13, 1955 (1980).

[3]W. Bociek and J. Lorenc, Phys. Rev. B 25, 2012 (1982) (preceding paper).

[4]M. V. Jarić, Ph.D. thesis (CUNY, New York, 1977) (unpublished).

[5]M. V. Jarić and J. L. Birman, Phys. Ref. B 16, 2564 (1977).

[6]Several typos occurred in Ref. 5: in the title "O_h^3-$Pm3n$" should be enclosed by parentheses; elsewhere in the text "G_0'" should be replaced by "G_1'"; at the beginning of Sec. III "O_h^3-$Pm3n(Pm3n)$" should read "(O_h^3-$Pm3n$)"; in the Table III, "$T^{1,2,6}$" should be replaced by "$T_h^{1,2,6}$"; in footnote 5, "Lavrenčić" should be replaced by "Lavrenčič."

[7]M. V. Jarić, Phys. Rev. B 23, 3460 (1981).

[8]The new criterion is called a "proposition" in Ref. 7, following a preprint form of Ref. 2. The development of various subduction criteria is also traced in Ref. 7.

[9]In rechecking calculations of Ref. 5, I discovered one transcriptional error: D_{2d}^4 was placed in the row with $i=1$ instead of $i=2$ [Table II, irreducible representations $^*\vec{X}(3)$ and $^*\vec{X}(4)$]. Thus, the subgroup S_4^1 is eliminated by CC and D_{2d}^4 becomes allowed [$S_4^1 \subset D_{2d}^4$, $i(S_4^1)=i(D_{2d}^4)=2$].

[10]In fact, Refs. 2 and 3 have not considered doubling in all three directions for X-point representations.