Landau's approach to symmetry changes in $A15$ (O_h^3-$Pm3n$) structure

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It is found that the results of Jarić and Birman of possible lower-symmetry phases arising from the $A15$ structure are not correct and, by using the Landau approach to symmetry changes at continuous phase transitions the corrected results for symmetry changes at $^*\vec{X}$ and $^*\vec{R}$ points of the Brillouin zone are presented.

Recently Jarić and Birman presented the results of an investigation of possible lower-symmetry groups which could arise from the O_h^3-$Pm3n$ group at $^*\vec{X}$ (cell doubling in one or two directions) and $^*\vec{R}$ (cell doubling in three directions) points of the Brillouin zone, and which seem to be relevant to the $A15$ structure.[1] Unfortunately, *their results are not correct* in the sense of the Landau approach to symmetry changes at continuous phase transitions.[2,3] In order to demonstrate this it is sufficient to restrict oneself only to the necessary condition for symmetry changes at a phase transition (having assumed it is continuous) which is, in fact, equivalent to the necessary condition for a minimum of the corresponding Landau thermodynamic potential within the original Landau approach.[4] This consists of considering *all essentially different* forms of the probability density vector $\delta\rho(\vec{r})$ which, as usually, can be written in the following form

$$\delta\rho(\vec{r}) = \sum_{i=1}^{d} c_i \varphi_i(\vec{r}) \tag{1}$$

where $\{\varphi_i;\ i=1,\ldots,d\}$ denotes a basis of the d-dimensional single-valued representation of the higher-symmetry group at a given point of the Brillouin zone and c_i's serve to construct independent invariants in the Landau thermodynamic potential. Then, by looking for all symmetry elements from the higher-symmetry group (O_h^3 in the case under consideration) that *leave those essentially different forms of* $\delta\rho(\vec{r})$ *invariant,* we find the lower-symmetry groups which could result from a continuous phase transition. The lower-symmetry groups obtained in this way, together with the corresponding ones obtained by Jarić and Birman are presented in Tables I, II, and III.

TABLE I. Phase transitions in O_h^3 based on $^*\vec{X}(m)$, $m=1,2,3,4$. Phases resulting from doubling in one direction. Representations are labeled according to Miller and Love, Ref. 5.

Representation	Subduction coefficient frequency, Ref. 1	Allowed subgroups of Jarić and Birman, Ref. 1	Allowed subgroups from the Landau approach
$^*\vec{X}(1)$	2	C_{2v}^1	C_{2v}^1
	1	D_{2h}^1, D_{2d}^5	D_{2h}^1, D_{2d}^5
$^*\vec{X}(2)$	2	C_{2v}^3	C_{2v}^3
	1	D_{2h}^3, D_{2d}^6	D_{2h}^3, D_{2d}^6
$^*\vec{X}(3)$ and $^*\vec{X}(4)$	2	D_2^2	D_2^2
	1	D_{2h}^5, $D_4^{3,7}$	D_{2h}^5, $D_4^{3,7}$

TABLE II. Phase transitions in O_h^3 based on $^*\vec{X}(m)$, $m=1,2,3,4$. Phases resulting from doubling in two directions (see Table I caption).

Representation	Subduction coefficient frequency, Ref. 1	Allowed subgroups of Jarić and Birman, Ref. 1	Allowed subgroups from the Landau approach
$^*\vec{X}(1)$	4	C_s^1	C_s^1
	3	C_{2v}^1	C_{2v}^1
	2	D_{2h}^1, C_{2v}^4	D_{2h}^1, C_{2v}^{16}
	1	D_{4h}^9, $D_{2h}^{3,5}$	D_{4h}^9
$^*\vec{X}(2)$	4	C_s^2	C_s^2
	3	C_{2v}^6	C_{2v}^6
	2	D_{2h}^4, C_{2v}^3	D_{2h}^4, C_{2v}^{17}
	1	D_{4h}^{11}, $D_{2h}^{3,7,8}$	D_{4h}^{11}
$^*\vec{X}(3)$ and $^*\vec{X}(4)$	4	D_2^3	D_2^3
	2	D_4^6, S_4^1, $D_{2h}^{9,11,13}$	D_4^6, D_{2h}^4, $D_{2h}^{9,11,13}$
	1	$D_{4h}^{13,15}$, $D_{2h}^{5,7,8}$	$D_{4h}^{13,15}$

TABLE III. Phase transitions in O_h^3 based on $^*\vec{R}(1)$, $^*\vec{R}(2) \oplus {}^*\vec{R}(3)$, and $^*\vec{R}(4)$. Representations are labeled according to Miller and Love, Ref. 5.

Representation	Subduction coefficient frequency Ref. 1	Allowed subgroups of Jarić and Birman, Ref. 1	Allowed subgroups from the Landau approach
$^*\vec{R}(1)$	2	$T^{1,4}$, $D_2^{2,3}$	T^2
	1	$T_h^{1,2,6}$, $O^{6,7}$ $D_{2h}^{3-14,16}$, $D_4^{3,4,7}$	O^4, T_h^3
$^*\vec{R}(2)$ $\oplus$ $^*\vec{R}(3)$	4	D_2^{1-4}	D_2^7
	2	D_{2h}^{1-16}, $D_4^{3,4,7,8}$	D_4^{10}, D_{2h}^{23}
$^*\vec{R}(4)$	6	C_1^1	C_1^1
	4	$C_2^{1,2}$	C_2^3
	3	$C_s^{1,2}$, C_i^1	C_2^3, C_s^3, C_i^1
	2	S_4^1, C_{2v}^{1-10}, $C_{2h}^{1,2,4,5}$, D_2^{1-4}, C_3^4	C_3^4, S_4^2, $D_2^{7,8}$, C_{2v}^{18}, C_{2h}^3
	1	D_3^7, C_{3i}^2, D_{2d}^{5-8}, D_{2h}^{1-16}, $D_4^{3,4,7,8}$, $C_4^{2,4}$	C_{3i}^2, D_3^7, D_4^{10}, D_{2d}^{11}, D_{2h}^{23}

Now, we can immediately notice disagreement with the results of Jarić and Birman (their allowed subgroups were obtained with the help of the chain subduction criterion). The reason is, that *the maximality principle* of Ascher[6] rather than the chain subduction criterion is *equivalent to a necessary condition for symmetry changes* at continuous phase transitions within the Landau approach,[7] where the form of $\delta\rho(\vec{r})$ plays a crucial role. Hence, our results are nothing but maximal epikernels of Ascher.

In addition, we note that the allowed subgroups from the Landau approach have to become subject to further restriction in the Landau thermodynamic theory; the corresponding c_i's in Eq. (1) have to realize a stable minimum of the Landau thermodynamic potential (being a function of c_i's).

[1]M. V. Jarić and J. L. Birman, Phys. Rev. B 16, 2564 (1977), and references cited therein.

[2]G. Ya. Lyubarski, *The Application of Group Theory in Physics* (Pergamon, Oxford, 1960).

[3]L. D. Landau and E. M. Lifshitz, *Statisticeskaja Fizika*, 3rd ed. (Nauka, Moscow, 1976).

[4]Note, however, that in the Landau thermodynamic potential coefficients connected with higher than second-order invariants in c_i's are, in general, functions of p and T, and from the necessary condition for minimum we find that some lower-symmetry phases can exist, if at all, only at a line on the p,T phase diagram; there is, so far, no experimental evidence for these cases.

[5]S. C. Miller and W. F. Love, *Irreducible Representations of Space Groups and Co-Representations of Magnetic Space Groups* (Pruett, Boulder, Colorado, 1967).

[6]E. Ascher, J. Phys. C 10, 1365 (1977).

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