LETTER TO THE EDITOR

On equitranslational continuous phase transitions

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Abstract. Ascher's tables of equitranslational phase transitions in crystals are augmented with tables providing the irreducible representations associated with each phase transition, and whether or not each of these irreducible representations satisfies the Landau stability criterion and the Lifshitz spatial homogeneity criterion.

A set of group theoretical criteria have been developed to predict the symmetry changes of a crystal arising from a continuous phase transition (Landau and Lifshitz 1980, Birman 1978, 1981). For a continuous phase transition between phases of space group symmetries G and H with order parameters associated with an irreducible representation $D_G^{(k,i)}$ of the space group G, the following four criteria have been used: (i) subduction criterion (Birman 1966); (ii) chain subduction criterion (Goldrich and Birman 1968, Jaric and Birman 1977); (iii) Landau stability criterion (Landau and Lifshitz 1980); and (iv) Lifshitz spatial homogeneity criterion (Landau and Lifshitz 1980).

Using the equivalent of the subduction and chain subduction criteria, Ascher (1977) has tabulated all possible changes in the symmetry of a crystal arising from a continuous phase transition for the case of equitranslational phase transitions: that is, for phase transitions between phases of space group symmetry G and H where both space groups contain the same subgroup of primitive translations. However, the irreducible representations associated with these phase transitions are not explicitly given, nor information as to whether or not these irreducible representations satisfy the Landau stability and the Lifshitz spatial homogeneity criteria. Such information is necessary when applying these tables to physical problems (Berenson *et al* 1982). In this Letter we provide the additional information to augment Ascher's tables, listing the irreducible representations associated with each equitranslational phase transition and whether or not these irreducible representations satisfy the Landau stability and Lifshitz spatial homogeneity criteria.

The irreducible representations associated with equitranslational phase transitions are $k = 0$ irreducible representations $D_G^{(0,1)}$ of the space group G. We denote each such irreducible representation by a symbol for the related irreducible representation of the point group of the space group G, using the symbols and enumeration of Koster *et al* (1963).

We give below a set of tables in the same numbering as Ascher's tables. In each table, to the right of the vertical lines, is the list of groups as given to the right of the vertical lines in Ascher's tables. To the left of each vertical line are the irreducible representations

Table 1.

${}^s\Gamma_1$	C_1

Table 2.

${}^s\Gamma_1$	C_2
Γ_2	C_1

${}^s\Gamma_1$	C_s
Γ_2	C_1

${}^s\Gamma_1^+$	C_i
Γ_1^-	C_1

Table 3.

${}^s\Gamma_1$	C_3
$({}^s\Gamma_2, {}^s\Gamma_3)^h$	C_1

Table 4.

${}^s\Gamma_1$	C_4
Γ_2	C_2
$(\Gamma_3, \Gamma_4)^h$	C_1

${}^s\Gamma_1$	S_4
Γ_2	C_2
$(\Gamma_3, \Gamma_4)^h$	C_1

Table 5.

${}^s\Gamma_1$	D_2
Γ_2	C_2
Γ_3	C_2
Γ_4	C_2

${}^s\Gamma_1$	C_{2v}
Γ_2	C_s
Γ_3	C_2
Γ_4	C_s

${}^s\Gamma_1^+$	C_{2h}
Γ_2^+	C_i
Γ_1^-	C_2
Γ_2^-	C_s

Table 6.

${}^s\Gamma_1$	C_6
Γ_4	C_3
$({}^s\Gamma_2, {}^s\Gamma_3)^h$	C_2
(Γ^5, Γ_6)	C_1

${}^s\Gamma_1$	C_{3h}
Γ_4	C_3
$({}^s\Gamma_2, {}^{\prime}\Gamma_3)^h$	C_s
(Γ_5, Γ_6)	C_1

${}^s\Gamma_1^+$	C_{3i}
Γ_1^-	C_3
$({}^s\Gamma_2^+, {}^s\Gamma_3^+)^h$	C_i
(Γ_2^-, Γ_3^-)	C_1

Table 7.

${}^s\Gamma_1^+$	C_{4h}
Γ_1^-	C_4
Γ_2^+	C_{2h}
Γ_2^-	S_4
(Γ_3^+, Γ_4^+)	C_i
(Γ_3^-, Γ_4^-)	C_s

Table 8.

${}^s\Gamma_1^+$	D_{2h}
Γ_1^-	D_2
Γ_4^+	C_{2h}
Γ_4^-	C_{2v}
Γ_3^+	C_{2h}
Γ_3^-	C_{2v}
Γ_2^+	C_{2h}
Γ_2^-	C_{2v}

Table 9.

${}^s\Gamma_1^+$	C_{6h}
Γ_1^-	C_6
Γ_4^+	C_{3i}
Γ_4^-	C_{3h}
$({}^s\Gamma_2^+, {}^s\Gamma_3^+)$	C_{2h}
(Γ_2^-, Γ_3^-)	C_2
(Γ_5^+, Γ_6^+)	C_i
(Γ_5^-, Γ_6^-)	C_s

Table 10.

${}^s\Gamma_1$	D_3
Γ_2	C_3
${}^s\Gamma_3^h$	C_2
${}^s\Gamma_3^h$	C_1

${}^s\Gamma_1$	C_{3v}
Γ_2	C_3
${}^s\Gamma_3$	C_s
${}^s\Gamma_3$	C_1

Table 11.

${}^{s}\Gamma_1$	D_4	${}^{s}\Gamma_1$	D_{2d}	${}^{s}\Gamma_1$	C_{4v}
Γ_2	C_4	Γ_2	S_4	Γ_2	C_4
Γ_3	D_2	Γ_3	D_2	Γ_3	C_{2v}
Γ_4	D_2	Γ_4	C_{2v}	Γ_4	C_{2v}
Γ_5	C_2	Γ_5^h	C_2	Γ_5	C_s
Γ_5	C_2	Γ_5^h	C_s	Γ_5	C_s
Γ_5	C_1	Γ_5^h	C_1	Γ_5	C_1

Table 12.

${}^{s}\Gamma_1$	T
$({}^{s}\Gamma_2, {}^{s}\Gamma_3)$	D_2
${}^{s}\Gamma_4^h$	C_3
${}^{s}\Gamma_4^h$	C_2
${}^{s}\Gamma_4^h$	C_1

Table 13.

${}^{s}\Gamma_1$	O	${}^{s}\Gamma_1$	T_d
Γ_2	T	Γ_2	T
${}^{s}\Gamma_3$	D_4	${}^{s}\Gamma_3$	D_{2d}
${}^{s}\Gamma_3$	D_2	${}^{s}\Gamma_3$	D_2
Γ_4	C_4	Γ_4	S_4
Γ_4	C_3	Γ_4	C_3
Γ_4	C_2	Γ_4	C_s
Γ_4	C_1	Γ_4	C_1
${}^{s}\Gamma_5^h$	D_2	${}^{s}\Gamma_5$	C_{2v}
${}^{s}\Gamma_5^h$	D_3	${}^{s}\Gamma_5$	C_{3v}
${}^{s}\Gamma_5^h$	C_2	${}^{s}\Gamma_5$	C_s
${}^{s}\Gamma_5^h$	C_1	${}^{s}\Gamma_5$	C_1

Table 14.

${}^{s}\Gamma_1$	D_6	${}^{s}\Gamma_1^+$	D_{3d}	${}^{s}\Gamma_1$	C_{6v}	${}^{s}\Gamma_1$	D_{3h}
Γ_2	C_6	Γ_2^+	C_{3i}	Γ_2	C_6	Γ_2	C_{3h}
Γ_3	D_3	Γ_1^-	D_3	Γ_4	C_{3v}	Γ_3	D_3
Γ_4	D_3	Γ_2^-	C_{3v}	Γ_3	C_{3v}	Γ_4	C_{3v}
${}^{s}\Gamma_6^h$	D_2	${}^{s}\Gamma_3^+$	C_{2h}	Γ_6	C_{2v}	Γ_6	C_{2v}
${}^{s}\Gamma_6^h$	C_2	${}^{s}\Gamma_3^+$	C_i	Γ_6	C_2	Γ_6	C_s
Γ_5^h	C_2	Γ_3^-	C_2	Γ_5	C_s	Γ_5	C_2
Γ_5^h	C_2	Γ_3^-	C_s	Γ_5	C_s	Γ_5	C_s
Γ_5^h	C_1	Γ_3^-	C_1	Γ_5	C_1	Γ_5	C_1

Table 15.

${}^{s}\Gamma_1^+$	D_{4h}
Γ_1^-	D_4
Γ_2^+	C_{4h}
Γ_2^-	C_{4v}
Γ_3^+	D_{2h}
Γ_3^+	D_{2d}
Γ_4^+	C_{2h}
Γ_4^-	D_{2d}
Γ_5^+	C_{2h}
Γ_5^+	C_{2h}
Γ_5^+	C_i
Γ_5^-	C_{2v}
Γ_5^-	C_{2v}
Γ_5^-	C_s

Table 16.

${}^{s}\Gamma_1^+$	T_h
Γ_1^-	T
$({}^{s}\Gamma_2^+, {}^{s}\Gamma_3^+)$	D_{2h}
(Γ_2^-, Γ_3^-)	D_2
${}^{s}\Gamma_4^+$	C_{2h}
${}^{s}\Gamma_4^+$	C_{3i}
${}^{s}\Gamma_4^+$	C_i
Γ_4^-	C_{2v}
Γ_4^-	C_3
Γ_4^-	C_s
Γ_4^-	C_i

Table 17.

${}^{s}\Gamma_1^+$	O_h	${}^{s}\Gamma_5^+$	C_{2h}
Γ_1^-	O	${}^{s}\Gamma_5^+$	C_i
Γ_2^+	T_h	Γ_4^-	C_{4v}
Γ_2^-	T_d	Γ_4^-	C_{2v}
${}^{s}\Gamma_3^+$	D_{4h}	Γ_4^-	C_{3v}
${}^{s}\Gamma_3^+$	D_{2h}	Γ_4^-	C_s
Γ_3^-	D_4	Γ_4^-	C_s
Γ_3^-	D_{2d}	Γ_4^-	C_1
Γ_3^-	D_2	Γ_5^-	D_{2d}
Γ_4^+	C_{4h}	Γ_5^-	C_{2v}
Γ_4^+	C_{3i}	Γ_5^-	D_3
Γ_4^+	C_{2h}	Γ_5^-	C_2
Γ_4^+	C_i	Γ_5^-	C_s
${}^{s}\Gamma_5^+$	D_{2h}	Γ_5^-	C_1
${}^{s}\Gamma_5^+$	D_{3d}		

Table 18.

${}^{s}\Gamma_1^+$	D_{6h}	Γ_6^-	D_2
Γ_1^-	D_6	Γ_6^-	C_{2v}
Γ_2^+	C_{6h}	Γ_6^-	C_2
Γ_2^-	C_{6v}	Γ_5^+	C_{2h}
Γ_3^+	D_{3d}	Γ_5^+	C_{2h}
Γ_3^-	D_{3h}	Γ_5^+	C_i
Γ_4^+	D_{3d}	Γ_5^-	C_{2v}
Γ_4^-	D_{3h}	Γ_5^-	C_{2v}
${}^{s}\Gamma_6^+$	D_{2h}	Γ_5^-	C_s
${}^{s}\Gamma_6^+$	C_{2h}		

associated with the equitranslational phase transitions read off of each row of Ascher's tables. Superscripts 's' and 'h' denote respectively that the irreducible representation does *not* satisfy the Landau stability criterion and the Lifshitz spatial homogeneity criterion. Physically irreducible representations (Lyubarskii 1960) are enclosed in parentheses.

For example, from Ascher's table 4 and table 4 below we have

${}^{s}\Gamma_1$	S_4	1	2
Γ_2	C_2	1	3
$(\Gamma_3, \Gamma_4)^h$	C_1	1	1.

Consequently, the equitranslational phase transitions $S_4^1 \rightarrow S_4^1$ and $S_4^2 \rightarrow S_4^2$ are associated with the irreducible representation Γ_1 which does not satisfy the Landau stability criterion; $S_4^1 \rightarrow C_2^1$ and $S_4^2 \rightarrow C_2^3$ are associated with Γ_2 which satisfies both the Landau stability and Lifshitz spatial homogeneity criteria; and $S_4^1 \rightarrow C_1^1$ and $S_4^2 \rightarrow C_1^2$ are associated with the physically irreducible representation (Γ_3, Γ_4) which does not satisfy the Lifshitz spatial homogeneity criterion.

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