Symmetry Properties of the Gallium Energy Bands. Effect of Spin-Orbit Interaction*

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The character tables for the double group corresponding to the space group (D_{2h}^{18}) are presented.

IN an earlier paper by Slater, Koster, and Wood,[1] the irreducible representations of the space group of the gallium structure (D_{2h}^{18}) were given. The degeneracies and the transformation properties of the states given there are those appropriate for problems, such as the solution of the one-electron Schrödinger equation in a periodic potential corresponding to gallium, where the effects of spin-orbit interactions are neglected. It is known[2] that if a term is added to the one-electron Hamiltonian of the form

$$(\hbar^2/4m^2c^2)(\mathbf{\Delta} V\times\mathbf{p}\cdot\boldsymbol{\delta}), \qquad (1)$$

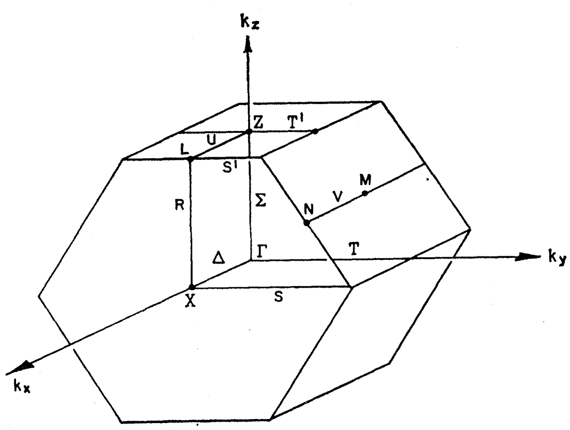

FIG. 1. Brillouin zone for the gallium structure.

corresponding to the interaction of the electron spin with the orbital motion, we must describe our states in terms of their transformation properties under the double group[3] corresponding to the space group D_{2h}^{18}. [In Eq. (1), V is the periodic potential, $\mathbf{p}$ the momentum of the electron, and $\boldsymbol{\delta}$ the spin operator.] This group has single-valued representations. These were those presented in reference 1. In addition, there are the double-valued representations to be used in discussions of the states corresponding to the motion of a single electron, where the effects of spin-orbit interaction are included. In this brief note, we present these additional double-valued representations. The reason for giving these additional representations is twofold. First they show the appropriate transformation properties of the states when spin-orbit interaction is included, and as a by-product, they show which degeneracies found in the single-valued representations would be removed if spin-orbit interaction was included.

In Fig. 1, for convenience, the Brillouin zone for the gallium structure is presented along with the notation for the various symmetry points in and on this zone. Before presenting the character tables for the additional representations of the D_{2h}^{18} double group, let us summarize the results of this note as far as the change in degeneracies are concerned in going from the case without spin-orbit interaction (reference 1) to the present case. In the work of Slater, Koster, and Wood, there were nondegenerate representations of the groups of the wave vector for all points in the interior and on the surface of the Brillouin zone, except for any point on the hexagonal face and any point along the line MNV. For these points the degeneracy was twofold. If we allow for the possibility of an electron having its spin up or down for each point in the zone, we see that these degeneracies are doubled. Thus, all of the points on the line MNV and any point on the hexagonal face would have a fourfold degeneracy and all other points in or on the zone would have a twofold degeneracy. When spin-orbit interaction is included the situation is modified

TABLE I. Characters of operations in groups of the wave vector at the points Γ, Z, X, and L. X_3 and X_4 are degenerate by time reversal as are L_3 and L_4.

	$\{\epsilon\|0\}$	$\{\delta_2^a\|\boldsymbol{\tau}\}$	$\{\delta_2^b\|0\}$	$\{\delta_2^c\|\boldsymbol{\tau}\}$	$\{i\|0\}$	$\{\sigma^a\|\boldsymbol{\tau}\}$	$\{\sigma^b\|0\}$	$\{\sigma^c\|\boldsymbol{\tau}\}$
Γ_5, Z_5	2	0	0	0	2	0	0	0
Γ_6, Z_6	2	0	0	0	-2	0	0	0
X_3, L_3	2	0	$2i$	0	0	0	0	0
X_4, L_4	2	0	$-2i$	0	0	0	0	0

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[1] J. C. Slater, G. F. Koster, and J. M. Wood, Phys. Rev. **126**, 1307 (1962).
[2] See, for example, R. J. Elliott, Phys. Rev. **96**, 280 (1954).
[3] For a discussion of the "double" space groups, their representations and further references see G. F. Koster, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1957) Vol. V, p. 173.

in the following way. All points in or on the Brillouin zone have a double degeneracy except the point M and the points on the XRL. These points have a fourfold degeneracy. (Just as in reference 1, some of these degeneracies come about only after time-reversal symmetry is included.[4]) Thus, the fourfold degeneracies at the points V, N and all points of the hexagonal face except the points on the line XRL are removed.

TABLE II. Characters of operations in the group of the wave vector at points Δ and U.

	$\{\epsilon\|0\}$	$\{\delta_2{}^a\|\boldsymbol{\tau}\}$	$\{\sigma^b\|0\}$	$\{\sigma^c\|\boldsymbol{\tau}\}$
Δ_5, U_5	2	0	0	0

TABLE III. Characters of operations in group of the wave vector at the points T, T', S, and S'. S_2 and S_4, S_3 and S_5, S_2 and S_4', S_3' and S_5' are degenerate by time reversal.

	$\{\epsilon\|0\}$	$\{\delta_2{}^b\|0\}$	$\{\sigma^a\|\boldsymbol{\tau}\}$	$\{\sigma^c\|\boldsymbol{\tau}\}$
T_5, T_5'	2	0	0	0
S_2, S_2'	1	i	i	1
S_3, S_3'	1	i	$-i$	-1
S_4, S_4'	1	$-i$	$-i$	1
S_5, S_5'	1	$-i$	i	-1

In Tables I–VI, we give the character tables for the points indicated in Fig. 1, and, in the captions to these tables, indicate the degeneracies that occur as a consequence of time reversal. (The notations used are the same as reference 1.) In order to conserve space we have not, in the tables, indicated the division of the group into classes, nor have we given the characters corresponding to the "barred operator." (These characters are just the negatives of those of the corresponding "unbarred operators".)

TABLE IV. Characters of operations in group of the wave vector at the points Σ and R. At the point R a pair of states transforming like R_5 will be degenerate with another pair transforming like R_5 by time reversal.

	$\{\epsilon\|0\}$	$\{\delta_2{}^c\|\boldsymbol{\tau}\}$	$\{\sigma^a\|\boldsymbol{\tau}\}$	$\{\sigma^b\|0\}$
Σ_5, R_5	2	0	0	0

TABLE V. Characters of operations in group of the wave vector at the points M and N. N_5 and N_6, N_7 and N_8 are degenerate by time reversal. At the point R a pair of states transforming like M_2 will be degenerate with another pair transforming like M_2 by time reversal.

	$\{\epsilon\|0\}$	$\{i\|0\}$	$\{\delta_2{}^a\|\boldsymbol{\tau}\}$	$\{\sigma^a\|\boldsymbol{\tau}\}$
M_2	2	0	0	0
N_5	1	1	1	1
N_6	1	1	-1	-1
N_7	1	-1	1	-1
N_8	1	-1	-1	1

TABLE VI. Characters of operations in group of the wave vector at the points H and V. H_3 and H_4, V_3 and V_4 are degenerate by time reversal.

	$\{\epsilon\|0\}$	$\{\sigma^a\|\boldsymbol{\tau}\}$
H_3	1	$\exp(i\mathbf{k}\cdot\boldsymbol{\tau})$
H_4	1	$-\exp(i\mathbf{k}\cdot\boldsymbol{\tau})$
	$\{\epsilon\|0\}$	$\{\delta_2{}^a\|\boldsymbol{\tau}\}$
V_3	1	$\exp(i\mathbf{k}\cdot\boldsymbol{\tau})$
V_4	1	$-\exp(i\mathbf{k}\cdot\boldsymbol{\tau})$

For all of the interior points of the Brillouin zone the character tables can be read directly from those of the irreducible representations of the point group of the group of the wave vector.[3] For all of the points of the surface, the technique of Sugita and Yamaka[5] was used to construct the representation of the group of the wave vector from those of the invariant symmorphic subgroup of half the order. In Table VII, we give the compatability tables which show how symmetries corresponding to special points go into those of neighboring points.

TABLE VII. Compatibility relations between irreducible representations for various symmetry points.

Γ_5	Γ_6	Z_5	Z_6			X_3	X_4
Δ_5	Δ_5	U_5	U_5			Δ_5	Δ_5
T_5	T_5	T_5'	T_5'			R_5	R_5
Σ_5	Σ_5	Σ_5	Σ_5			S_2	S_4
						S_3	S_5
$\underline{L_3}$	$\underline{L_4}$	$\underline{T_5}$		$\underline{N_5}$	$\underline{N_6}$	$\underline{N_7}$	$\underline{N_8}$
U_5	U_5	T_5'		H_4	H_3	H_3	H_4
R_5	R_5						
S_2'	S_4'						
S_3'	S_5'						
$\underline{R_5}$		$\underline{M_2}$		$\underline{S_2}$	$\underline{S_3}$	$\underline{S_4}$	$\underline{S_5}$
H_3		V_3		H_3	H_4	H_4	H_3
H_4		V_4					

[5] T. Sugita and E. Yamaka, Reports of the ECL, NTT (Japan) 2, No. 8, 5 (194).