A NOTE ON THE DERIVATION OF MAGNETIC LATTICES

T. S. G. KRISHNAMURTY AND P. GOPALAKRISHNAMURTY
Andhra University, Waltair

It is well known that crystals are classified into 230 space groups belonging to one or the other of the 14 Bravais lattices and the 32 crystal classes. To account for the magnetic properties of crystals it was found necessary to introduce the time reversal operation $\mathcal{R}$. The introduction of this new operation increases the number of the point groups from 32 to 122, the Bravais lattices from 14 to 36 and the space groups from 230 to 1651. The additional double-coloured magnetic Bravais lattices have been derived by Zamorzaev[1] using a mathematical method and also by Belov, Neronova and Smirnova[2] using the fundamental property of coloured translations while Villain's[3] approach in his paper on magnetic lattices has been quite different. Employing the concept of a semi-direct product (Lomont,[4] and Altmann[5]) of two groups, Opechowski and Guccione[6] have shown that only 22 distinct magnetic double-coloured Bravais lattices exist. Recently Bhagavantam and Pantulu[7] deduced them as variants of the translational groups. In this note it is proposed to establish a close connection between the magnetic Bravais lattices and the stars of the wave vectors of the symmorphic space groups (point space groups) given in the *International Tables for X-ray Crystallography*.[8] It is shown here how some of the double-coloured magnetic Bravais lattices can be straightaway read off from the stars of the symmorphic space groups and from the definition of the semi-direct product of two groups the other dichromatic magnetic Bravais lattices are related to the stars of the appropriate point space groups.

It has been shown by the authors[9] that the non-equivalent alternating representations of a group G induce the distinct magnetic variants of G. If G is now taken as a translational group T corresponding to a Bravais lattice, the total symmetric representation of T will induce the conventional (uncoloured) Bravais lattice. The other real one-dimensional irreducible representations (alternating representations) of T induce the double-coloured magnetic Bravais lattices, which are otherwise known as the magnetic variants of the Bravais lattices.

Two magnetic double-coloured Bravais lattices T_{m1} and T_{m2} of respective magnetic holohedries H_1 and H_2 are said[6] to belong to the same magnetic Bravais class (which are hereafter designated as equivalent) if (*i*) the semi-direct product of T_{m1} and H_1 is isomorphous to that of T_{m2} and H_2 and (*ii*) the uncoloured elements of the former semi-direct product under this isomorphism correspond to those of the latter. This definition will be applied in obtaining the magnetic variants of the Bravais lattices in two and three dimensions from the alternating representations of the appropriate translational group.

For the derivation of the magnetic variants of the lattices in two dimensions, it is sufficient[9] to consider the translational group generated by the elements T_x and T_y such that $T_x^2 = T_y^2 = E$ (identity). Thus the translational group in two dimensions will have 4 real one-dimensional representations. Each alternating representation of the translational group induces a double-coloured magnetic lattice and is associated with a non-zero wave vector $\vec{k}$ (k_x, k_y) of the reciprocal space, since the generating elements T_x and T_y can be represented respectively by exp. $(2\pi i k_x)$ and exp. $(2\pi i k_y)$ (Koster[10]). The character table of the translational group in two dimensions is

Wave vector	E	T_x	T_y	T_xT_y	Magnetic Bravais lattice
(0, 0)	1	1	1	1	..
(0, ½)	1	1	−1	−1	T_{m1}
(½, 0)	1	−1	1	−1	T_{m2}
(½, ½)	1	−1	−1	1	T_{m3}

The magnetic variants of the Bravais lattices in two dimensions will be now enumerated and described in terms of the stars of the symmorphic plane space groups.

(1) *Monoclinic*.—The magnetic holohedries of the three magnetic lattices T_{m1}, T_{m2} and T_{m3} are the same and consist of the identity E and the complementary symmetry operation i (Zheludev[11]). From the definition of the semi-direct product it may be seen that T_{m1}, T_{m2} and T_{m3} are all equivalent. Hence only one distinct variant of the monoclinic lattice exists and the three wave vectors (0, ½), (½, 0) and (½, ½) may be regarded as equivalent.

These three wave vectors are contained in the stars b, c and d respectively of the two-dimensional monoclinic primitive point space group p2 (p. 58*) which has the holohedral symmetry of the system. Thus the stars b, c and d of the space group are equivalent and any one of them can be taken to induce the magnetic variant of the lattice.

(2) *Orthorhombic Primitive.*—To enumerate the distinct magnetic variants of this lattice, the symmorphic space group *pmm* (p. 61) is considered whose underlying point group has the orthorhombic holohedry (D_{2h}). The magnetic holohedry[12] of the magnetic lattice T_{m1} is $\mathbf{E}$, C_z, σ_x, σ_y and that of T_{m2} is $\mathbf{E}$. C_z, σ_x, σ_y. But the magnetic holohedries of T_{m1} and T_{m2} are isomorphous and different from that of T_{m3} which consists of E, C_z, σ_x, σ_y. It can be shown from the idea of the semi-direct product that T_{m1} is equivalent to T_{m2} but different from T_{m3}. Thus the stars b and c of the space group *pmm* are equivalent and different from the star d. Hence there are only two magnetic variants of the orthorhombic primitive lattice.

In this way the magnetic variants of the other Bravais lattices for the remaining systems can be obtained by noting that (*i*) only those symmorphic space groups whose underlying point group is the holohedry of the system have to be taken into account, (*ii*) components of the wave vectors in the stars of the symmorphic space groups, which are given with respect to the crystallographic axes in the case of the derived lattices, should be transformed to the Bravais axes to decide equivalence among the stars, (*iii*) if two or more of the wave vectors $(0, \frac{1}{2})$, $(\frac{1}{2}, 0)$ and $(\frac{1}{2}, \frac{1}{2})$ occur in a star of a point space group, then the corresponding alternating representations of the translational group will get clubbed together so that they can be regarded as degenerate and (*iv*) only those stars containing any one of the three wave vectors need alone be considered.

(3) *Orthorhombic Derived.*—The magnetic variant of this lattice is due to the star b of the space group *cmm* (p. 64).

(4) *Tetragonal.*—The star b of the space group *p4m* (p. 66) gives rise to the magnetic variant.

(5) *Hexagonal.*—No variant exists in this case since the wave vectors $(0, \frac{1}{2})$, $(\frac{1}{2}, 0)$ and $(\frac{1}{2}, \frac{1}{2})$ occur in the star c of the space group *p6m* (p. 72).

THREE-DIMENSIONAL MAGNETIC BRAVAIS LATTICES

The distinct magnetic variants corresponding to each one of the 14 conventional Bravais lattices of the 7 crystal systems are obtained below on the lines similar to those adopted in the derivation of the magnetic variants of the two-dimensional lattices described earlier. The character table of the translational group in three dimensions, generated by the elements T_x, T_y and T_z such that $T_x^2 = T_y^2 = T_z^2 = \mathbf{E}$ (identity operation), is given below:

Wave vector	E	T_x	T_y	T_z	T_xT_y	T_xT_z	T_yT_z	$T_xT_yT_z$	Magnetic lattice
$(0, 0, 0)$	1	1	1	1	1	1	1	1	..
$(\frac{1}{2}, 0, 0)$	1	−1	1	1	−1	−1	1	−1	T_{m1}
$(0, \frac{1}{2}, 0)$	1	1	−1	1	−1	1	−1	−1	T_{m2}
$(0, 0, \frac{1}{2})$	1	1	1	−1	1	−1	−1	−1	T_{m3}
$(\frac{1}{2}, \frac{1}{2}, 0)$	1	−1	−1	1	1	−1	−1	1	T_{m4}
$(\frac{1}{2}, 0, \frac{1}{2})$	1	−1	1	−1	−1	1	−1	1	T_{m5}
$(0, \frac{1}{2}, \frac{1}{2})$	1	1	−1	−1	−1	−1	1	1	T_{m6}
$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	1	−1	−1	−1	1	1	1	−1	T_{m7}

(1) *Triclinic.*—The magnetic holohedry consisting of the elements E and i is the same for all the seven magnetic lattices T_{m1}, T_{m2} .., T_{m7}. Thus all the seven alternating representations of the translational group in this case are equivalent giving rise to only one magnetic variant of the lattice. So in the symmorphic space group $P\bar{1}$ (p. 75), the stars b, c, d, e, f, g and h are all equivalent and the magnetic variant can be taken to be due to any one of these seven stars.

(2) *Monoclinic Primitive.*—The point space group to be considered is P2/m (p. 91). The magnetic holohedries of T_{m4}, T_{m6} and T_{m7} are isomorphous and those of T_{m1}, T_{m3} and T_{m5} are also isomorphous. Thus the three magnetic variants will be due to the stars d (or c or g), e (or f or h) and b.

(3) *Monoclinic Side-Centered.*—The point space group C2/m (p. 95) is chosen. The wave vectors $(\frac{1}{2}, 0, 0)$ and $(0, \frac{1}{2}, 0)$ occur in the star e while $(\frac{1}{2}, 0, \frac{1}{2})$ and $(0, \frac{1}{2}, \frac{1}{2})$ are present in the star f. From the definition of the semi-direct product, the magnetic lattices T_{m3} and T_{m7} can be shown to be equivalent. Hence the magnetic variants of the lattice are due to the stars b and c (or d).

(4) *Orthorhombic Primitive.*—The space group to be selected is *Pmmm* (p. 133). The

* Page numbers given in brackets against the space groups refer to the *International Tables for X-ray Crystallography*, 1952.

stars (e, b, c) are equivalent and so do the stars (f, g, d). The stars h, e (or b or c) and f (or g or d) will give rise to the three variants of the lattice.

(5) *Orthorhombic Body-Centered*.—The symmorphic space group I*mmm* (p. 163) is to be taken. Its reciprocal space group is F*mmm* (p. 159). The magnetic variants of the body-centered lattice will be now associated with the wave vectors of F*mmm*. On transformation of the components of the wave vectors of F*mmm* from the crystallographic axes to the Bravais axes it is found that the wave vectors $(0, 0, \frac{1}{2})$ and $(\frac{1}{2}, \frac{1}{2}, 0)$ belong to the star c, $(0, \frac{1}{2}, 0)$ and $(\frac{1}{2}, 0, \frac{1}{2})$ to the star d and $(\frac{1}{2}, 0, 0)$ and $(0, \frac{1}{2}, \frac{1}{2})$ to the star c of the space group F*mmm*. Thus the only variant of the body-centered orthorhombic lattice is due to the star b $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ of F*mmm*.

(6) *Orthorhombic Face-Centered*.—The required space group is F*mmm* (p. 159). The reciprocal symmorphic space group is I*mmm* (p. 163). Effecting the transformation to the Bravais axes, the wave vectors $(\frac{1}{2}, 0, 0)$, $(0, \frac{1}{2}, 0)$, $(0, 0, \frac{1}{2})$ and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ belong to the star k of I*mmm*. It can be shown on lines similar to the magnetic variants of the triclinic lattice that the stars b, c and d of I*mmm* are all equivalent so that only one magnetic variant is permitted.

(7) *Orthorhombic Side-Centered*.—The point space group to be regarded is C*mmm* (p. 154). The wave vectors $(\frac{1}{2}, 0, \frac{1}{2})$ and $(0, \frac{1}{2}, \frac{1}{2})$ belong to the star f and $(\frac{1}{2}, 0, 0)$ and $(0, \frac{1}{2}, 0)$ belong to the star e. Thus the three variants are due to the stars b, c and d.

(8) *Tetragonal Primitive*.—The space group to be chosen is P4/*mmm* (p. 213). The three magnetic variants of this lattice are due to the stars b, c and d as can be easily seen from the *International Tables*.

(9) *Tetragonal Body-Centered*.—In this case the space group to be dealt with is I4/*mmm* (p. 241). The wave vectors $(\frac{1}{2}, 0, 0)$, $(0, \frac{1}{2}, 0)$, $(0, 0, \frac{1}{2})$ and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ correspond to the star f and the wave vectors $(\frac{1}{2}, 0, \frac{1}{2})$, and $(0, \frac{1}{2}, \frac{1}{2})$ belong to the star c. Hence the only variant is due to the star b.

(10) *Rhombohedral (Trigonal)*.—The space group under question is P$\bar{3}$1 *m* (p. 268). The variant of the lattice is due to the star b while the remaining wave vectors belong to the stars g and f of the space group.

(11) *Hexagonal*.—It can be easily read off from the *International Tables* that the only permitted variant in this case is due to the star b of the space group P6/*mmm* (p. 298).

(12) *Cubic Primitive*.—The resulting magnetic variant of the lattice is due to the star b of the space group P*m*3*m* (p. 330).

(13) *Cubic Body-Centered*.—The space group considered here is I*m*3*m* (p. 344) whose reciprocal symmorphic space group is F*m*3*m* (p. 338) and the magnetic variant of the cubic body-centered lattice is due to the star b of F*m*3*m*.

(14) *Cubic Face-Centered*.—Since the reciprocal point space group I*m*3*m* (p. 344) of the space group F*m*3*m* (p. 338) does not contain a star which consists of only one of the seven wave vectors $(0, 0, \frac{1}{2})$, $(\frac{1}{2}, 0, 0)$, etc., there is no magnetic variant of the cubic face-centered lattice.

The magnetic variants of a Bravais lattice are described in terms of the stars of a symmorphic space group which belongs to the Bravais lattice and whose underlying point group symmetry is the holohedry of the system and those of the derived lattices are expressed in terms of the stars of the reciprocal symmorphic space groups. It may be further noted that the choice of the stars may be restricted to those that contain only one wave vector which necessarily has the holohedral symmetry of the system. Other stars having more than one wave vector need not be considered in the derivation of the magnetic lattices as they possess lower symmetry.

The novelty in this investigation paves the way for the construction of the Shubnikov space groups from the representation theory of the conventional space groups.

The authors wish to express their gratitude to Prof. T. Venkatarayudu for the stimulating and clarifying discussions which they had with him on the problem.

1. Zamorzaev, A. M., *Soviet Phys. Cryst.*, 1957, **2**, **10**.
2. Belov, N. V., Neronova, N. N. and Smirnova, T. S., *Ibid.*, 1957, **2**, 311.
3. Villain, J., *Phys. Chem. Solids*, 1959, **11**, 303.
4. Lomont, J. S., *Applications of Finite Groups*, Academic Press, New York, 1959, p. 29.
5. Altmann, S. L., *Rev. Mod. Phys.*, 1963, **35**, 641.
6. Opechowski, W. and Guccione, R., *Magnetism*, Academic Press, Oxford, 1965, **2 A**, pp. 105.
7. Bhagavantam, S. and Pantulu, P. V., *Proc. Ind. Acad. Sci.*, 1966, **63**, 391.
8. Norman, F. M., Henry and Lonsdale, K., *International Tables for X-ray Crystallography*, 1952, **1**.
9. Krishnamurty, T. S. G. and Gopalakrishnamurty, P., A paper on "Magnetic Symmetry Groups," communicated to *Acta Cryst.*, 1968.
10. Koster, G. F., *Solid State Physics*, Academic Press, 1957, **5**, 173.
11. Zheludev, I. S., *Soviet Phys. Crystall.*, 1960, **5**, 328.
12. Bhagavantam, S., *Crystal Symmetry and Physical Properties*, Academic Press, London, 1966, p. 51.