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Crystal Lattices and Sub-Lattices.

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1. Introduction.

Various molecular theories of crystal elasticity employ a common assumption, introduced by Born [1], to relate changes in molecular configurations to macroscopic deformation. Briefly, we select as a reference some homogeneous configuration of a crystal, together with a choice of reference lattice vectors E_a ($a = 1, 2, 3$). If the crystal undergoes a homogeneous deformation, with deformation gradient F, the assumption is that the vectors e_a, given by

$$(1) \qquad\qquad e_a = FE_a ,$$

are a possible set of lattice vectors for the deformed crystal. In some types of phase transitions, the assumption fails, if we adhere to a strict interpretation of the phrase « lattice vectors ». Illustrative examples of some of the subtleties which can occur are covered by Parry [2], for example. In the transitions which he treats, and various others, one can continue to use (2), by adopting a more liberal interpretation of « lattice vectors ». With some reason, crystallographers tend to be somewhat finicky about terminology, so it seems preferable to introduce another name for the vectors which have some, but not all the properties of lattice vectors; I will refer to them as « sub-lattice

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vectors ». My purpose is to explain what they are, and to present some elementary theory of relations between different sets of lattice and sub-lattice vectors.

2. The vectors.

For purposes of illustration, we accept the classical idea of a crystal configuration of a body filling all of space. As a matter of definition, it must have a periodic structure, describable by a translation group T. That is, if r_0 is the position vector of any point, T generates a countable set of points which are physically indistinguishable from it. Here, T is representable as follows: for some choice of constant and linearly independent (lattice) vectors e_a, the points generated are those which can be represented in the form

$$(2) \qquad r_N = r_0 + n_N^a e_a , \qquad N = 1, 2, 3, ...,$$

where we use the summation convention. The components n_N^a must be integers, and every choice of integers is to be included. Two translation groups are equivalent if they generate exactly same points. It then follows easily, and is well-known that, for this, it is necessary and sufficient that these exist integers m_b^a, with

$$(3) \qquad \det m = \pm 1 , \qquad m = \| m_b^a \| ,$$

such that the corresponding lattice vectors are related by

$$(4) \qquad \bar{e}_b = m_b^a e_a .$$

As a matter of convention, the lower index will label rows, in such matrices. Such matrices form a group G under matrix multiplication or, if you prefer, under composition of mappings of the form (4). Since G consists of sets of integers, it is discrete. That it is infinite and not compact follows from that fact that it includes all matrices of the form

$$(5) \qquad \begin{Vmatrix} 1 & n & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{Vmatrix},$$

where n is any integer.

Any set of lattice vectors determines a (maximal) point group P, a subgroup of the orthogonal group. An orthogonal transformation Q is included in it, provided that there exists some $m \in G$ such that

$$(6) \qquad\qquad Q e_a = m_a^b e_b \, .$$

Subgroups of P are also counted as point groups. All this is standard, used in Seitz's [3] discussion of the crystallographic groups, for example. As is discussed by Ericksen [4], every point group is conjugate to a finite subgroup of G and *vice versa*.

In the above discussion, something is left unsaid, although some might consider it to be understood. For the rather idealistic homogeneous amorphous solid, our translation groups would serve to generate physically equivalent points, for any choice of the e_a, and the crystallographer does not mean to include such things. Roughly, what he has in mind is that our translation groups should be maximal, in some sense. For simplicity, I ignore modern attempts to relax definitions to include odd materials which have some type of crystallinity, but don't fit the classical definition of crystals, such as some of the smectic liquid crystals. To see how to make this more precise, we presume that there is a preferred equivalence class of translation groups, related by G, the maximal groups. Let f_a be a set of vectors which generates some translation group, so that, as before,

$$(7) \qquad\qquad r_N = r_0 + n_N^a f_a$$

generates points physically equivalent to the (arbitrary) point r_a. The idea is that a maximal group should generate all of these points, and possibly more. Let e_a be the lattice vectors for a maximal group. Then r_N, given by [7] must also be representable in the form

$$(8) \qquad\qquad r_N = r_0 + \bar{n}_N^a e_a \, .$$

In (7), the n_N^a must include all possible integers, but $\bar{n}_N^a$ need not take on all such values. By choosing special values of n_N^a, we see that we must have, for some integers p_a^b

$$(9) \qquad\qquad f_a = p_a^b e_b \, ,$$

where $p = \| p_a^b \|$ is a matrix of integers, not necessarily in G, but with

non-zero determinant, since the f_a are to be linearly independent. Also, if (9) holds, we have

$$\text{(10)} \qquad\qquad \bar{n}_N^a = n_N^o p_o^a ,$$

giving integers $\bar{n}_N^a$ for every choice of integer n_N^o, so no other conditions need hold. When p is unimodular, hence included in G, we stay in the aforementioned equivalence class. When f_a does not generate a maximal group, that is when $|\det p| > 1$, it and $\bar{f}_a$ generate the same point sets, if they are related by G. I expect that crystallographers would object to calling all such vectors lattice vectors, and such terminology could well cause confusion. Thus, I will call them *sub-lattice* vectors. With this background, we restate these propositions:

i) Lattice vectors e_a, $\bar{e}_a$, *etc.* generate the equivalence class C of maximal translation groups. We can generate C by applying all transformations in G to one set of lattice vectors, in the manner indicated by (4).

ii) Sub-lattice vectors f_a can be obtained by applying a transformation of the type (9) to any set of lattice vectors, with $|\det p| > 1$. Sub-lattice vectors f_a and $\bar{f}_a$ are regarded as equivalent, when one can be obtained from the other by applying a transformation in G.

Actually, practice is somewhat variable, and sub-lattice vectors are, on occasion, used as lattice vectors. For example, a monatomic crystal might be described as being a body-centered cubic, suggesting lattice vectors which are orthogonal, identifiable with the edges of the cube. In our terminology, these are sub-lattice vectors. A set of lattice vectors can be obtained by using two of the edges issuing from one corner, plus the vector connecting the corner to the center of the cube.

It is easy to see, and known, that the maximal point group for a set of lattice or sub-lattice vectors is not changed, if we replace the vectors by an equivalent set. In the example just mentioned, the indicated lattice and sub-lattice vectors generate the same point group. However, in general, the point group for a set of lattice vectors differs from that for a set of sublattice vectors. For example, if we have orthogonal lattice vectors with $\|e_1\| = \|e_2\| = \|e_3\|$, P includes the 90° rotation

$$\text{(11)} \qquad Qe_1 = e_2 , \qquad Qe_2 = -e_1 , \qquad Qe_3 = e_3 .$$

A possible set of sub-lattice vectors is

(12) $f_1 = 2e_1, \quad f_2 = e_2, \quad f_3 = e_3.$

Applying Q to these, we get

(13) $Qf_1 = 2f_2, \quad Qf_2 = -\tfrac{1}{2}f_1, \quad Qe_3 = e_3,$

and, because of the occurrence of the factor $-\tfrac{1}{2}$, this is not in the point group determined by f_a. Similarly, the point group for a set of sublattice vectors can include orthogonal transformations not belonging too the point group for lattice vectors. It is reasonable to expect that lattice vectors give a better estimate of the true symmetry of a crystal, and I know no reason to doubt this. Thus, some dangers are involved, in blurring the distinction between lattice and sublattice vectors.

To restate remarks made in the introduction, there are cases where the kinematical assumption (1) fails to apply if we use lattice vectors, but applies if we use selected subsets of sub-lattice vectors. Clearly, one then must use care, in properly accounting for crystal symmetries.

3. Simple observations.

In the following, we consider any fixed configuration of a crystal, so the equivalence class C of lattice vectors is fixed. In describing the relations between different sets of sub-lattice and lattice vectors, we encounter another group, the group R of non-singular matrices which are rational numbers. Its significance is made clear by the following easy

THEOREM 1. *If $\bar{f}_a$ and f_a are any two sets of sub-lattice vectors, we have*

(14) $\bar{f}_a = r_a^b f_b \quad r \in R.$

Conversely, if $r \in R$, there exist two sets of sub-lattice vectors such that (14) holds.

PROOF. If $\bar{f}_a$ and f_a are sub-lattice vectors, and e_a is any set of lattice vectors, we have matrices of integers $\bar{p}$ and p, with $|\det \bar{p}| > |$

and $|\det p| > |$ such that

(15) $$\bar{f}_a = \bar{p}_a^b e_b\,, \qquad f_a = p_a^b e_b\,.$$

eliminating e_a between these equations gives (14), with

(16) $$r = \bar{p} p^{-1}\,.$$

Conversely, if $r \in R$, we can write its entries in the form

$$r_b^a = \bar{p}_b^a / q\,,$$

where $\bar{p}_b^a$ and q are integers, since a set of rationals has a common denominator. By multiplying numerator and denominator by an integer, if necessary, we can arrange that $q > 1$ and $\det \|\bar{p}_b^a\| > 1$. Then, if e_a is any set of lattice vectors,

$$\bar{f}_a = \bar{p}_a^b e_b$$

and

$$f_a = q e_a$$

give two sets of sub-lattice vectors, with

$$\bar{f}_a = r_a^b f_b\,. \qquad \text{QED.}$$

For a crystal with atomic structure, it might be easy to spot a set of sub-lattice vectors, not immediately obvious whether these are lattice vectors. In dealing with such questions, I have found useful some classical theorems in algebra, adopted below.

THEOREM 2. *Suppose f_a are sub-lattice vectors. Then there exists a set of lattice vectors $\bar{e}_a$ such that*

(17)
$$\begin{cases} f_1 = n_1 \bar{e}_1\,, \\ f_2 = n_2 \bar{e}_1 + n_3 \bar{e}_2\,, \\ f_3 = n_4 \bar{e}_1 + n_5 \bar{e}_2 + n_6 \bar{e}_3\,, \end{cases}$$

where the n's are integers, with $|n_2| < |n_1|$, $|n_4| < |n_1|$, $|n_5| < |n_3|$.

PROOF. If e_a are any set of lattice vectors, there is an integer matrix p such that

$$(18) \qquad f_a = p_a^b e_b .$$

If $\bar{e}_b$ is another set of lattice vectors, we have

$$(19) \qquad e_a = m_a^b \bar{e}_b , \qquad m \in G$$

It then follows that

$$(20) \qquad f_a = \bar{p}_a^b \bar{e}_b ,$$

where

$$(21) \qquad \bar{p} = pm .$$

It then remains to show that, given p, we can find $m \in G$ so that $\bar{p}$ takes the form indicated by (17). This follows from a result attributed to Hermite by Mac Duffee [4, Theorems 103.4 and 103.5].   QED.

Essentially the same proof yields.

THEOREM 3. *Suppose e_a and f_a are given sets of lattice and sub-lattice vectors. Then, there exists a set of sub-lattice vectors $\bar{f}_a$ which are equivalent to f_a, such that*

$$(22) \qquad \begin{cases} \bar{f}_1 = n_1 e_1 , \\ \bar{f}_2 = n_2 e_1 + n_3 e_2 , \\ \bar{f}_3 = n_4 e_1 + n_5 e_2 + n_6 e_3 , \end{cases}$$

with $|n_2| < |n_1|, \ |n_4| < |n_1|, \ |n_5| < |n_3|$.

Somewhat similar is

THEOREM 4. *Suppose e_a and f_a are lattice and sub-lattice vectors. Then there exist lattice vectors $\bar{e}_b$ and sub-lattice vectors $\bar{f}_a$ which are equivalent to f_a, with*

$$(23) \qquad \begin{cases} \bar{f}_1 = n_1 \bar{e}_1 , \\ \bar{f}_2 = n_2 \bar{e}_2 , \\ \bar{f}_3 = n_3 \bar{e}_3 , \end{cases}$$

where the n's are integers such that n_1 is a divisor of n_2 and n_2 is a divisor of n_3.

PROOF. From the hypothesis, we must have

$$f_a = p_a^b e_b \,,$$

where p is a matrix of integers. The conclusion follows if we can show that there exist matrices m and $\bar{m}$, both in G, such that $\bar{m}pm$ has the indicated diagonal form. This follows immediately from Mac Duffee's [5] Theorem 105.2.   QED.

If we modify (1), to allow use of sub-lattice vectors, it would take the form

(24) $$f_a = FF_a \,,$$

F_a referring to some reference set. If we replace F_a by an equivalent set

$$\overline{F}_a = m_a^b F_b \,, \quad m \in G,$$

then it becomes

$$\bar{f}_a = F\overline{F}_a \,,$$

with

$$\bar{f}_a = m_a^b f_b \,,$$

equivalent to f_a. Using Theorem 4, we can find reference lattice vector E_a such that

$$F_a = n^a E_a \quad \text{(no sum)},$$

if the F_a are properly chosen. We can then rewrite (24) in the equivalent form

$$f_a = n^a F E_a \quad \text{(no sum)},$$

and one can use Theorem 1 to introduce lattice vectors e_a which are rather simply related to f_a. In the particular cases treated by Parry [2], the final relations can be put in the form

(26) $$e_1 = FE_1 \,, \quad e_2 = FE_2 \,, \quad e_3 = 2FE_3 \,,$$

For F taking the crystals from a body-centered phase, to a phase which is not body-centered.

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