We first show that the integers f, g and h determine the group $C_f \times C_{fg} \times C_{fgh}$. First we write fgh as a product of distinct primes $p_1^{e_{13}} p_2^{e_{23}} \dots p_k^{e_{k3}}$, $e_{13} > 0$. Then fg can be written in the form $p_1^{e_{12}} p_2^{e_{22}} \dots p_k^{e_{k2}}$, where $0 \le e_{l2} \le e_{l3}$. Finally, $f = p_1^{e_{11}} p_2^{e_{21}} \dots p_k^{e_{k1}}$, and $0 \le e_{l1} \le e_{l2} \le e_{l3}$. The order of the group $C_f \times C_{fg} \times C_{fgh}$ is then $f^3 g^2 h = n = p_1^{e_1} p_2^{e_2} \dots p_k^{e_k}$, where $e_l = e_{l1} + e_{l2} + e_{l3}$.

If a and b are relatively prime then the direct product of the cyclic groups C_a and C_b of orders a and b is isomorphic to the cyclic group C_{ab} of order ab. Therefore

$$C_f = C_{p_1^{e_{11}}} \times C_{p_2^{e_{21}}} \times \dots \times C_{p_k^{e_{k1}}},$$
$$C_{fg} = C_{p_1^{e_{12}}} \times C_{p_2^{e_{22}}} \times \dots \times C_{p_k^{e_{k2}}},$$

and

$$C_{fgh} = C_{p_1^{e_{13}}} \times C_{p_2^{e_{23}}} \times \dots \times C_{p_k^{e_{k3}}}.$$

Since the factors in a direct product commute, we have

$$C_f \times C_{fg} \times C_{fgh} = (C_{p_1^{e_{11}}} \times C_{p_1^{e_{12}}} \times C_{p_1^{e_{13}}}) \times (C_{p_2^{e_{21}}} \times C_{p_2^{e_{22}}} \times C_{p_2^{e_{23}}}) \times \dots \times (C_{p_k^{e_{k1}}} \times C_{p_k^{e_{k2}}} \times C_{p_k^{e_{k3}}}).$$

The integers e_{ij} are called the invariants of the group. A basic theorem in group theory says that an Abelian group is completely characterized by its invariants, from which our assertion follows.

It follows that to enumerate the classes of equivalent derivative lattices of index n, we need to know the number of ways each e_l can be written as a sum of three non-negative integers e_{l1}, e_{l2}, e_{l3} with $0 \le e_{l1} \le e_{l2} \le e_{l3} \le e_l$. Let $n_3(e_l)$ represent this number. Then, since the partitions of the e_l are independent, any one can be combined with any other. Thus the number of ways of writing L/L' as a direct product of three cyclic groups is equal to the product $n_3(e_1) \dots n_3(e_k)$.

This argument can easily be modified to hold for lattices in any dimension d.

Example: Let L be a two-dimensional lattice and L' a sublattice of index $n = 2^3 \times 5^4 \times 7 \times 11^2$. In dimension 2, $e_l = e_{l1} + e_{l2}$ and so $e_{l2} = e_l - e_{l1}$. Assuming $0 \le e_{l1} \le e_{l2} \le e_l$, we obtain the following formula for $n_2(e_l)$:

$$n_2(e_l) = \begin{cases} (e_l + 1)/2 & \text{if } e_l \text{ is odd} \\ e_l/2 + 1 & \text{if } e_l \text{ is even.} \end{cases}$$

Thus $n_2(3) = 2$, $n_2(4) = 3$, $n_2(1) = 1$ and $n_2(2) = 2$. The product of these numbers is 12, so there are twelve classes of derivative lattices of index $n = 2^3 \times 5^4 \times 7 \times 11^2$.

Unfortunately there is no simple formula* for $n_d(e_l)$ except in the case $d = 2$. However, there is no difficulty in calculating $n_d(e_l)$ by hand if e^l is not too large (or by computer if it is).

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* *Note added in proof:* See, however, Kucab (1981).

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Bragg's Law in Higher Dimensions

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Abstract

Incommensurate modulated structures are no longer 'perfect' crystals in $\mathbb{E}^3$, where $\mathbb{E}^n$ is the n-dimensional affine Euclidian space; on the other hand they are crystals in $\mathbb{E}^4$, $\mathbb{E}^5$ or $\mathbb{E}^6$ whose cell is obtained from the experimental diffraction pattern in $\mathbb{E}^{*3}$. But Bragg's law is more general and it is shown that hyperplane incident waves are diffracted by sets of lattice hyperplanes of perfect crystals of $\mathbb{E}^n$.

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Introduction

Incommensurate modulated structures such as γ-Na_2CO_3 (Van Aalst, Den Hollander, Peterse & de Wolf, 1976), $K_2Pt(CN)_4Br_{0.3}.xH_2O$ (Comes, Lambert, Launois & Zeller, 1973; Comes, Lambert & Zeller, 1973), TaS_2 (Williams, Parry & Scruby, 1975; Brouwer & Jellinek, 1974), $Fe_{1-x}O$ (Andersson & Sletnes, 1977; Yamamoto, Nakazawa & Tokonami, 1979) no longer have translational periodicity in $\mathbb{E}^3$.

If we use one, two or three more dimensions, these modulated structures recover a translational periodicity and consequently are crystals* in $\mathbb{E}^4$, $\mathbb{E}^5$ or $\mathbb{E}^6$. In these superspaces we define the translation lattice from the complete experimental diffraction pattern which consists of Bragg reflections and their satellites (de Wolf, 1974, 1977; Janner & Janssen, 1977).

On the other hand, the Ewald construction for crystal diffraction has been generalized to a special four-dimensional space where the space–time symmetries are considered (Janner & La Fleur, 1971). It will be useful for the description of diffraction phenomena in the one-phonon case or when the crystal is placed in a monochromatic laser field or a sound wave.

But the von Laue and Bragg laws are still more general because we can consider in $\mathbb{E}^4$ the diffraction of monochromatic hyperplane waves by crystals and further the extension to $\mathbb{E}^n$.

Sets of lattice hyperplanes in a perfect crystal of $\mathbb{E}^n$

Let a perfect crystal be of $\mathbb{E}^n$, one simple cell $(O\mathbf{a}_1 \dots \mathbf{a}_n)$ of which is chosen as a basis of $\mathbb{E}^n$.

The lattice points† are joined together in sets of parallel equidistant lattice rows, planes and hyperplanes ‡ – (hk) in $\mathbb{E}^2$, (hkl) in $\mathbb{E}^3$, $(hklm)$ in $\mathbb{E}^4$, $(h_1 \dots h_n)$ in $\mathbb{E}^n$ – represented by the following equations: §

$$\left.\begin{array}{ll} xh + yk = \sigma & \text{in } \mathbb{E}^2 \\ xh + yk + zl = \sigma & \text{in } \mathbb{E}^3 \\ xh + yk + zl + tm = \sigma & \text{in } \mathbb{E}^4 \\ x^1h_1 + \dots + x^nh_n = \sigma & \text{in } \mathbb{E}^n. \end{array}\right\} \quad (1)$$

Miller indices $hklm$, $h_1 \dots h_n$ are relative integers without a common divisor and $\sigma = \dots -2, -1, 0, +1, +2, \dots$. We write d_{hk}, d_{hkl}, d_{hklm}, $d_{h_1 \dots h_n}$ for the interhyperplanar spacings, *i.e.* the equidistances between two nearest rows, planes or hyperplanes of the set: for example, it is the distance between the hyperplane which contains origin O $(\sigma = 0)$ and the nearest one (for example $\sigma = +1$) which intersects axes $x^1, \dots x^n$ at points $A_1, \dots, A_n$, with $OA_1 = a_1/h_1, \dots, OA_n = a_n/h_h$. See Fig. 1 where a concrete example in $\mathbb{E}^4$ is represented.

* Definition of a perfect crystal in $\mathbb{E}^n$: an infinite object whose Abelian group of all the translations that leave it unchanged as a whole is isomorphic to $\mathbb{Z}^n$, $\mathbb{Z}$ being the additive group of all the relative integers (Weigel & Berar, 1978).

† We recall that the elements $\mathbf{t} = u^1\mathbf{a}_1 + \dots + u^n\mathbf{a}_n$, where $n^1, \dots, n^n$ are all the n-tuplets of relative integers. The ends of vectors $\mathbf{t}$ are the nodes or the points of the lattice.

‡ The hyperplanes of $\mathbb{E}^n$ are $(n-1)$-dimensional spaces $\mathbb{E}^{n-1}$ in $\mathbb{E}^n$. So a straight line is a hyperplane of $\mathbb{E}^2$, a plane is a 'hyperplane' of $\mathbb{E}^3$, *etc.*

§ In $\mathbb{E}^3$ $\mathbf{OX} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$ and so it is unavailing to write equation (1) as $xh/a + yk/b + zl/c = \sigma$.

Diffraction of monochromatic hyperplane waves by a crystal in $\mathbb{E}^n$

Let monochromatic hyperplane waves W_0 of wave-vector $\mathbf{k}_0$ be incident upon a crystal in $\mathbb{E}^n$ (see Figs. 2 and 3), where $\mathbf{k}_0 = 2\pi\mathbf{S}_o/\lambda_0$: $\mathbf{S}_0$ is the unit vector in the incident direction and λ_0 is the wavelength. So the wave fronts are straight lines in $\mathbb{E}^2$, planes in $\mathbb{E}^3$ and hyperplanes in $\mathbb{E}^4, \dots, \mathbb{E}^n$.

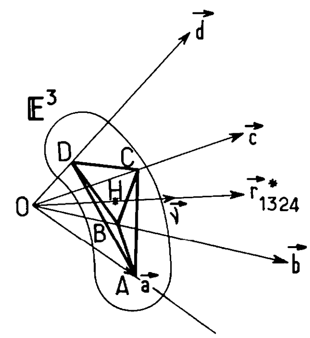

Fig. 1. O **abcd** is a cell of hexaclinic crystal in $\mathbb{E}^4$. The space $\mathbb{E}^3$, which contains the tetrahedron $ABCD$, is the hyperplane nearest to origin O among the set (1, 3, 2, 4) of the lattice hyperplanes in this crystal (in this case: $OA = a$, $OB = b/3$, $OC = c/2$ and $OD = d/4$). Point H is the intersection of hyperplane $\mathbb{E}^3$ with the straight line drawn from O and orthogonal to $\mathbb{E}^3$: so $OH = d_{1324}$.

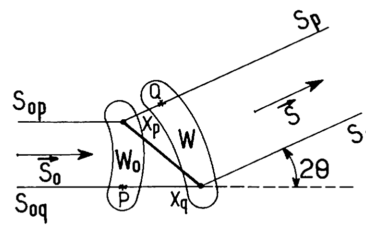

Fig. 2. Scattering in $\mathbb{E}^n$ of hyperplane waves W_0 by two centers X_p and X_q. If $n = 4$, W_0 and W are three-dimensional spaces.

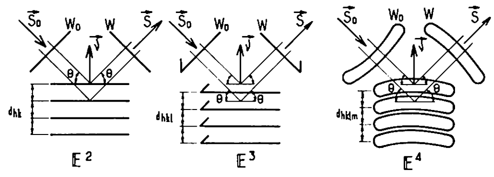

Fig. 3. Bragg's law in $\mathbb{E}^2$, $\mathbb{E}^3$ and $\mathbb{E}^4$ (or $\mathbb{E}^n$).

If we suppose that the waves W_0 are elastically† scattered by the points of the crystal lattice, they will be diffracted in the direction of unit vector **S** by a set of lattice hyperplanes $(h_1 \ldots h_n)$ if the following necessary condition, generalized von Laue's law, is verified.

$$\mathbf{s} = \frac{\mathbf{S} - \mathbf{S}_0}{\lambda_0} = \mathbf{r}^*_{h_1 \ldots h_n} = h_1 \mathbf{a}^{1*} + \ldots + h_n \mathbf{a}^{n*}, \quad (2)$$

where the vectors $\mathbf{a}^{1*}, \ldots \mathbf{a}^{n*}$ are defined by the relations $\mathbf{a}_i . \mathbf{a}^{j*} = \delta^j_i$ (Kronecker symbols), *i.e.* $(\mathbf{a}^{*1}, \ldots, \mathbf{a}^{*n})$ is the dual basis (in $\mathbb{E}^{*n}$) of the basis $(\mathbf{a}_1, \ldots, \mathbf{a}_n)$ of $\mathbb{E}^n$, and $h_1 \ldots h_n$ are the Miller indices of the set $(h_1 \ldots h_n)$.

Proof: see Fig. 2: X_p and X_q are two scattering centers in the crystal. S_{0p} and S_{oq} are two rays of the incident parallel beam meeting X_p and X_q. The incident wave W_0 at X_p–orthogonal to $\mathbf{S}_o$–intersects S_{0q} at point P. S_p and S_q are two rays of the scattered parallel beam starting from X_p and X_q. The wave‡ W scattered by X_q–orthogonal to **S**–intersects S_p at point Q.

The ray striking X_q travels a longer distance than the ray striking X_p; the difference is $PX_q - X_pQ = \mathbf{X}_p\mathbf{X}_q (\mathbf{S} - \mathbf{S}_0)$ and the corresponding phase difference is $-\boldsymbol{\Delta}\mathbf{k} . \mathbf{X}_p\mathbf{X}_q$, where $\boldsymbol{\Delta}\mathbf{k} = \mathbf{k} - \mathbf{k}_0 = 2\pi(\mathbf{S} - \mathbf{S}_0)/\lambda_0 = 2\pi\mathbf{s}$.

The proof can be continued in exactly the same way as in $\mathbb{E}^3$. Bragg's law is

$$\|\mathbf{s}\| = \|\mathbf{r}^*_{h_1 \ldots h_n}\|. \quad (3)$$

So it only agrees with part of the necessary conditions for diffraction (2).

In fact, as in $\mathbb{E}^3$, we have $s = 2 \sin \theta / \lambda_0$, where 2θ is the angle between $\mathbf{S}_0$ and **S** and $r^*_{h_1 \ldots h_n} \times d_{h_1 \ldots h_n} = 1$ (see theorem).

So, Bragg's law can also be written, as it usually is,

$$\lambda_0 = 2 d_{h_1 \ldots h_n} \sin \theta_{h_1 \ldots h_n}. \quad (3')$$

Theorem: $\mathbf{r}^*_{h_1 \ldots h_n}$ is orthogonal to the lattice hyperplanes $(h_1 \ldots h_n)$ and $r^*_{h_1 \ldots h_n} \times d_{h_1 \ldots h_n} = 1$.

Proof in $\mathbb{E}^n$: (1) Let the hyperplane $(h_1 \ldots h_n)$ meet the origin O. The coordinates of the general point X $(x^1 \ldots x^n)$ of this hyperplane verify (1) with $\sigma = 0$. Therefore,

$$\mathbf{OX} . \mathbf{r}^*_{x_1 \ldots h_n} = (x^i \mathbf{a}_i) . (h_j \mathbf{a}^{*j}) = x^i h_i = 0$$

according to (1). Of course, the two sums over i and j, from 1 to n, are understood according to Einstein's convention. Consequently, $\mathbf{r}^*_{h_1 \ldots h_n}$ is orthogonal to $(h_1 \ldots h_n)$.

(2) Let us generalize Fig. 1 to space $\mathbb{E}^n$: the spacing $d_{h_1 \ldots h_n} = OH$ is the orthogonal projection of the vector $\mathbf{OA}_l$ on the straight line which supports the normal to $(h_1 \ldots h_n)$ whose $\mathbf{v}$ is the unit vector; therefore

$$d_{h_1 \ldots h_n} = OH = \mathbf{OA}_l . \mathbf{v} = \frac{\mathbf{OA}_l . \mathbf{r}^*_{h_1 \ldots h_n}}{r^*_{h_1 \ldots h_n}}$$

$$= \frac{\mathbf{a}_l . r^*_{h_1 \ldots h_n}}{h_l r^*_{h_1 \ldots h_n}} = \frac{1}{r^*_{h_1 \ldots h_n}}.$$

Remark: the second-, third-, *etc.* order reflections upon the set of lattice hyperplanes $(h_1 \ldots h_n)$, where $h_1 \ldots h_n$ are relative integers without any common divisor, are included in Bragg's law such as is written in (3′) if we also use the fictitious sets $(2h_1 \ldots 2h_n)$, $(3h_1 \ldots 3h_n)$, *etc.*, where the spacings $d_{2h_1 \ldots 2h_n}$ equal $d_{h_1 \ldots h_n}/2$ *etc.*

Conclusion

We have proved in this paper that the monochromatic hyperplane waves of $\mathbb{E}^n$ are diffracted by the lattice hyperplanes of a perfect crystal according to the generalized von Laue law which contains the generalized Bragg law. Note that von Laue's and Bragg's original laws in $\mathbb{E}^3$ are special cases of those discussed here.

† Elastically means that the wavelength λ of the scattered waves W equals λ_0.

‡ It is more correct to write that W is the hyperplane tangential (orthogonal to **S**) to the spherical wave scattered by X_q.

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