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Importance of reciprocal space in crystallographic study

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Abstract

It is one of the foundational geometric and mathematical concepts in crystallography for analyzing crystal and interpretation of crystal structure. The construction of mathematical relationship between reciprocal lattice and real unit cells and the application of Edward sphere to visualize Laue diffraction methods. The importance of this space is across many crystallographic methods like X-ray diffraction and in the analysis of complex structural features.The high-speed computing has enhanced the ability to predict complex crystal structures.

Keywords: *Reciprocal space, Crystallography, Edward sphere, Diffraction*

Introduction:

purpose of this study is to provide an introduction to several of general importance and the aspects of reciprocal space. We first summarize the basic definitions and aspects of crystallography, while the concept of the reciprocal lattice. This introductory section is followed by a summary of the basic relationships between the direct and associated reciprocal lattices. We then introduce the elements of tensor-algebraic formulation of such dual relation applications of emphasis those that are important in many applications of reciprocal space to crystallographic algorithms. We proceed with a section that demonstrates the role of mutually reciprocal bases in transformations of coordinates c and conclude with a brief outline of some important analytical aspects of reciprocal space, most of which are further developed in other parts.

Reciprocal lattice in crystallography: The notion of mutually reciprocal triads of vectors dates back to the introduction of vector calculus by J. Willard Gibbs in the 1880s (eg. Wilson, 1901). This concept appeared to be useful in the early interpretations of diffraction from single crystals (Ewald, 1913; Laue, 1914) and its first detailed exposition and the recognition of its importance in crystallography can be found in Ewald's (1921) article. The following free translation of Ewald's (1921) introduction, presented in a somewhat different notation, may serve the purpose of this section. To the set of there corresponds in the vector calculus a set of 'reciprocal vectors' h, which are defined (by Gibbs) by the following properties

$$a_i - b_k = 0 (i \neq k) \quad (1)$$

And $$a_i - b_i = 1 \quad (2)$$

where i and k may each equal 1, 2 or 3.

The first equation says that each vector by is perpendicular to two vectors a,, as follows from the vanishing scalar products. Equation 2 provides the norm of m of the vector by the length of this vector must be chosen such that the projection of bi on the direction of has the length 1/ai, where ai is the magnitude of the vector a, rather The consequences of equations (1) and (2) were elaborated by Ewald (1921) and are very well documented in the subsequent literature, crystallographic as well as other.

As is well known, the reciprocal lattice occupies prominent position in crystallography and there are nearly as many accounts of its importance as there are crystallographic texts. It is not intended to review its applications, in any detail, in the present section; this is done in the remaining chapters and sections of the present volume.

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It seems desirable, however, to mention by way of an introduction some fundamental geometrical, physical and mathematical aspects of crystallography, and try to give a unified. demonstration of the usefulness of mutually reciprocal bases as an interpretive tool. Consider the equation of a lattice plane in the direct lattice. It is shown in standard textbooks (e.g. Buerger, 1941) that this equation. is given by

$$hx+ky+lz=n \qquad (3)$$

where h. k and I are relatively prime integers (ie. not having a common factor other than +1or -1, known as Miller indices of the lattice plane other than the coordinates of any point lying in the plane and are expressed as fractions of the magnitudes of the basis vectors a, b and e of the direct lattice, respectively, and w is an integer denoting the serial number of the lattice plane family of parallel and equidistant (4) planes, the inter to the spacing being denoted by day; value corresponds to (hkl) plane passing through the origin.Consider r=xa+yb+zc and rL = ua+ vb+wc, where u, v, w are any integers, denote the position vectors of the point xyz and a lattice point uvw lying in the plane, respectively, and assume that r and rL are different vectors. If the plane denoted by N. where N is proportional to the vector product of two in-plane lattice vectors, the vector product of the equation of the lattice vector fro the equation of the lattice plane becomes

$$N-(r-r_L)=0 \quad \text{or} \quad N-r=N-r_L \qquad (4)$$

N-For equations (3) and (4) to be identical, the plane normal N must satisfy the requirement that $N-r_L=n$, where is an (unrestricted) integer. Let us now consider the basic diffraction relations (e.g. Lipson & Cochran, 1966). Suppose a parallel beam of monochromatic radiation, of wavelength A, falls on a lattice of identical point scatterers. If it is assumed that the scattering is elastic, ie. there is no change of the wavelength during this process, the wave vectors the incident and scattered radiation have the same magnitude, which can conveniently be taken as $1/\lambda$. A consideration of path and phase differences between the waves outgoing from two point scatterers separated by the lattice vector r, (defined as above) shows that the condition for their maximum constructive interference is given by

$$(S-S0)r_L= n \qquad (5)$$

where so and s are the wave vectors of the incident and scattered beams, respectively, and a is an arbitrary integer. Since r_L=ua+vb+we, where a, v and w are unrestricted integers, equation (5) is equivalent to the equations of Laue:

$$h.a = h, \quad h.b = k \quad , h.c = l \qquad (6)$$

where $h = S - S_0$ is the diffraction vector, and h, k and I are integers corresponding to orders of diffraction from the three-dimensional lattice (Lipson & Cochran, 1966). The diffraction vector thus has to satisfy a condition that is analogous to that imposed on the normal to a lattice plane. The next relevant aspect to be commented on is the Fourier expansion of a function having the periodicity of the crystal lattice. Such functions are e.g. the electron density, the density of nuclear matter and the electrostatic potential in the crystal, which are the operative definitions of crystal structure in X-ray, -ray, neutron and electron-diffraction methods of crystal structure determination. A Fourier expansion of such a periodic function may be thought of as a related superposition of waves (e.g. Buerger, 1959), with wavevectors related to the interplanar spacings d, in the crystal lattice. Denoting the wavevector of a Fourier wave by g (a function of hkl), the phase of the Fourier wave at the point r in the crystal is given by $2\pi g.r$, and the triple Fourier series corresponding to the expansion of the periodic function, say G(r), can be written as

$$G(r) = \Sigma C(g)\exp(-2xig-r) \qquad (7)$$

where C(g) are the amplitudes of the Fourier waves, or Fourier coefficients, which are related to the experimental data. Numerous examples of such expansions appear throughout this volume. The permissible wavevectors in the above expansion are restricted by the periodicity of the function G(r). Since, by definition, G(r) = G(r+ rL) where r_L is a direct-lattice vector, the right-) must remain unchanged when r is replaced by $r+r_L$This, however, can be true only if the scalar product g.rL is an integer. Each of the above three aspects of crystallography may lead, independently, to a useful introduction of the reciprocal vectors, and there are many examples of this in the literature. It is interesting, however, to consider the representation of the equation

$$v.r_L = n \qquad (8)$$

which is common to all three, in its most convenient form. Obviously, the vector v which stands for the plane normal, the diffraction vector, and the wave vector in a Fourier expansion, may still be referred to any permissible basis and so may r, by an appropriate transformation. Suppose v = UA + VB + WC where A, B and C are linearly Let independent vectors. Equation (8) can then be written as

$$(UA+VB+WC).(ua+vb+wc) = n, \qquad (9)$$

or, in matrix notation,

$$\begin{pmatrix} U & V & W \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix} . \begin{pmatrix} a & b & c \end{pmatrix} \begin{pmatrix} u \\ v \\ w \end{pmatrix} = n \qquad (10)$$

$$\begin{pmatrix} U & V & W \end{pmatrix} \begin{pmatrix} A.a & A.b & A.c \\ B.b & B.b & B.c \\ C.a & C.c & C.c \end{pmatrix} \begin{pmatrix} u \\ v \\ w \end{pmatrix} = n \qquad (11)$$

The simplest representation of equation (8) results when the matrix of scalar products in (11) reduces to a unit matrix. This can be achieved (i) by choosing the basis vectors ABC to be orthonormal to the basis vectors abc, while requiring that the components of r, be integers, or (ii) by requiring that the bases ABC and abc coincide with the same orthonormal basis, ie. expressing both v and r_L in (8), in the same Cartesian system. If we choose the first alternative, it is seen that the components of the vector v, and hence those of N, h and g, are of necessity integers, since u, v and w are already integral. The components of v include Miller indices, in the case of the lattice plane, they coincide with the orders of diffraction from a three-dimensional lattice of scatterers, and correspond to the summation indices in the triple Fourier series (7). The basis vectors A, B and C are reciprocal to a, b and c, as can be seen by comparing the scalar products in (11) with those in (1) and (2). In fact, the bases ABC and abc are mutually reciprocal. Since there are no restrictions on the integers U, V and W, the vector v belongs to a lattice which, on account of its basis, is called the reciprocal lattice.

It follows that, at least in the present case, algebraic simplicity goes together with ease of interpretation, which certainly accounts for much of the importance of the reciprocal lattice in crystallography. The second alternative of reducing the matrix in (11) to a unit matrix, a transformation of (8) to a Cartesian system, leads to non-integral components of the vectors, which makes any interpretation of v or r, much less transparent. However, transformations to Cartesian systems are often very useful in crystallographic computing and will be discussed. We shall, in what follows, abandon all the temporary notation used above and write the reciprocal-lattice vector

$$h = ha^* + kb^* + lc^* \qquad (12)$$

$$h = h_1 a^1 + h_2 a^2 + h_3 a^3 = \sum_{i=1}^{3} h_i a^i \qquad (13)$$

denote the direct-lattice vectors by r_L = ua + vb + wc as above, or by

$$r_L = u^1 a_1 + u^2 a_2 + u^3 a_3 = \sum_{i=1}^{3} u^i a_i$$

The representations (13) and (14) are used in the tensor- algebraic formulation of the relationships between mutually reciprocal bases.

Conclusion:

The reciprocal space provides a frame work for the diffraction patterns of a crystal in which good peaks represent the Miler indices,intensity of peaks gives information about size, shape and surface quality. It enhances crystallographic phase quality more than real space methods by utilizing an explicit likelihood function.

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Conflicts of interest

The authors declare that there are no conflicts of interest regarding the publication of this paper

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