American Mineralogist, Volume 63, pages 840–846, 1978

How much crystallography should we teach geologists?

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Abstract

A crystallography course, consisting of 24 lectures and 12 three-hour laboratory periods, is shown to cover the foundations of morphological as well as structural crystallography. It is meant to give the entering geology student the basic crystallographic understanding on which to build the solid knowledge of minerals without which no study of rocks is conceivable. Facing his overwhelming responsibility, the crystallography teacher in a geology department must select his topics with extreme care and strive to impart the know-why as well as the know-how. A realistic goal is to bring the student to a point where he can: *morphologically*, get all information from the external form (to be able to find the morphological space group of a euhedral crystal) and, *structurally*, understand how a crystal structure is built and how it can be solved by diffraction (to be able to build a crystal-structure model after studying a structure paper in the literature).

Introduction

The teaching of crystallography is on the decline in geology departments the world over, a fact which hardly needs documentation in a volume dedicated to two retiring professors of Harvard University who will leave very much of a vacancy cluster in crystallography–mineralogy in their department. Among numerous other universities where retiring crystallographers have not been replaced by specialists in their field are Massachusetts Institute of Technology, The Johns Hopkins University, and the University of California, Berkeley. In Europe too, crystallography is now being taught to geologists more and more by non-crystallographers who devote a few lectures to the subject matter which they "have picked up along the way."

The purpose of this paper is to point out how much crystallography, classical as well as X-ray, can be taught to geology students in as few as 24 lectures and 12 laboratory periods, the length of a "semester" in Canada. Since all geologists will deal with crystalline matter for the duration of their professional lives, it should be possible to convince the profession that these few hours are well spent by their students. The course to be described assumes that the students have had the equivalent of freshman chemistry, physics, and mathematics. At McGill University crystallography is a required course for entering geology students who have had their science preparation in a two-year junior college program[1]. The failure rate in the course is about 9.6 percent: 19 students out of 197 have had to repeat the course in the last eight years.

Textbook and laboratory manual

Finding a textbook for the course is an unsolved problem. The ideal textbook should be directed to future geologists; it should therefore cover crystal morphology and crystal structure (crystal optics too, although at McGill as in many other schools the optical part of crystallography is taught later in the curriculum, just before optical mineralogy); it should present the most basic concepts *in depth* despite, or rather because of, the short time allotted to the course (the smattering technique, which relies on such subterfuges as putting the name of the new concept to be introduced between quotation marks in lieu of explanation or definition and expecting results to be memorized without first having been proved, has been particularly sterile in teaching crystallography).

Among the books that cover the desired topics, we may mention one in French by Van Meerssche and Feneau-Dupont (1973) (750 p.) and two in Italian, by

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[1] This province-wide program was established about ten years ago by the provincial government; it follows eleven grades of schooling and leads to a 3-year bachelor's program.

Bonatti and Franzini (1972) (361 p.) and by Rigault (1976) (215 p.). In English the book by Sands (1969) (165 p.) has been reviewed in this journal (v. *56,* p. 641); it is of the right size, but it is written for chemistry students. We have nevertheless selected it and are supplementing it with a 32-page syllabus on morphology (Donnay and Donnay, 1972), together with short appendices on fundamentals that need brushing up and material not easily accessible: (a) spherical trigonometry and vector algebra (4 p.); (b) derivation of the 32 crystallographic point groups (5 p.); (c) twinning (7 p.); (d) complex numbers; (e) intensities of diffracted beams (2 p.). The students buy their *Laboratory Manual* (Donnay and Donnay, 1973) (67 p.), which comes with plastic copies of five X-ray films and four charts used to read the films. The Manual contains ten assignments, which follow a model one, on "Significant Figures," demonstrating how to fill in such recurring sections as: results obtained, conclusions, discussion, problems (which have to be solved), and suggestions (requested from the student) for improving the given assignment.

The first part of the course: morphological crystallography

The first half of the term deals with classical crystallography, including the Bravais-Mallard-Friedel theory of twinning; the second half treats X-ray crystallography. The standard definitions of a crystal, pre- and post-1912, open the first lecture: "a chemically homogeneous solid, wholly or partly bounded by natural planes that intersect at predetermined angles" *vs.* "any solid in which an atomic pattern is repeated periodically in three dimensions, that is, any solid that diffracts an incident X-ray beam." These definitions are elaborated upon, with illustrations of physical and chemical properties of crystalline matter that depend on its periodicity—the lattice. Discontinuous vectorial properties, such as growth velocity, when plotted in all directions around a point, yield representative surfaces characterized by sharp minima in directions normal to faces. The chemical formula of a mineral, no matter how complicated it looks, can be rewritten with small integral subscripts once the structure type is known and the elements are properly grouped.

Table 1. Simplified nomenclature of the 47 crystal forms

The 32 noncubic forms: (The adjectives give the shape of the right section of the form near its apex.)		Nonpolar forms, with two polar components turned through θ with respect to each other:			
		$\theta \neq 1/2$ period		$\theta = 1/2$ period	
Monohedron	Parallelohedron	...		...	
Dihedron		Rhombic tetrahedron		Tetragonal tetrahedron	
Trigonal	pyramids prisms dipyramids	Trigonal	trapezohedra	Rhombohedron	
Rhombic		...		Rhombic	scalenohedra
Tetragonal		Tetragonal		...	
Ditrigonal		...		Ditrigonal	
Hexagonal		Hexagonal		...	
Ditetragonal		...		...	
Dihexagonal		...		...	

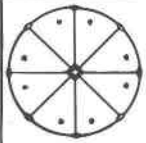
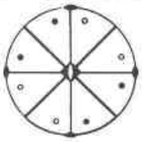
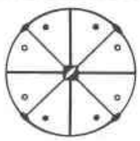
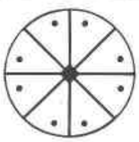
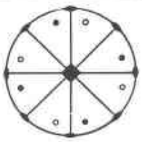
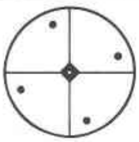
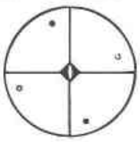
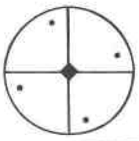
The 15 cubic forms: (The prefixes recall the face shape in the lone form.)

Cube = Hexahedron	Rhombdodecahedron		Tetra (Octa) hedron*
↓			↓ ↓
Dihexahedron =	Pentagondodecahedron	Trigon Tetragon Pentagon	tritetra (octa) hedron*
↓	↓		↓ ↓
Tetrahexahedron	Didodecahedron		Hexatetra (octa) hedron*

*Read "Tetrahedron" or "Octahedron": the derivation is the same for both.

The second lecture introduces students to symmetry elements and symmetry operations of the point-group kind, which they observe on wooden models in their first laboratory assignment. The symmetry *of a crystal* is *defined* as "the symmetry common to all of its properties"; the Neumann "principle" is unmasked as a "definition", incorrectly described throughout the literature—a shock and eye-opener to all young students! Another definition introduced here is that of a group, so the students can appreciate the fact that symmetry operations do form groups: point groups or space groups (the latter are introduced later in the term). In the second laboratory assignment the students learn the nomenclature (Table 1) of the 32 non-cubic and the 15 cubic forms and assign the point-group symmetry (from the list of Hermann-Mauguin symbols on the board) to wooden models and to a few well-developed euhedral crystals. The third laboratory assignment, "Derivation of the crystal forms in every point group by means of stereographic projections," helps the students to become thoroughly familiar with symmetry operations, symmetry elements, crystal faces, crystal forms, and point groups, bringing together, as it does, all the new concepts introduced thus far. Double-entry tables are provided on separate sheets for the various crystal systems; each table has as many columns of stereographic circles as there are point groups in the system, each column being headed by the proper Hermann-Mauguin point-group symbol. Below the column heading, the first circle shows the symmetry elements in this point group. The rows of the table represent the possible crystal forms, beginning with the general form {*hkl*} and ending with the most specialized form of lowest multiplicity. Colored pencils are used to underline primary, secondary, and tertiary symmetry elements in the Hermann-Mauguin symbol and to color the corresponding Gadolin symbols in the top circle. On each successive circle the student fills in the face poles of one of the various forms that are possible in the point group. For each crystal system an accom-

Table 2. Crystal forms in the tetragonal system*

	Holohedry	Hemihedries					Tetartohedries	
	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$	$\bar{4}\,2\,m$	$\bar{4}\,m\,2$	$4\,m\,m$	$4\,2\,2$	$\frac{4}{m}$	$\bar{4}$	4
Form symbol h>k								
hkl	ditetragonal dipyramid 16 1	tetragonal scalenohedron 8 1	tetragonal scalenohedron 8 1	ditetragonal pyramid 8 1	tetragonal trapezohedron 8 1	tetragonal dipyramid 8 1	tetragonal tetrahedron 4 1	tetragonal pyramid 4 1
h0l	tetragonal dipyramid 8 ·m·	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 8 1	tetragonal tetrahedron 4 ·m·	tetragonal pyramid 4 ·m·	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 8 1	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 8 hkl 1	$\bar{4}\,m\,2$ 4 hkl 1	$4\,m\,m$ 4 hkl 1
hhl	tetragonal dipyramid 8 ··m	tetragonal tetrahedron 4 ··m	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 8 1	tetragonal pyramid 4 ··m	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 8 1	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 8 hkl 1	$\bar{4}\,2\,m$ 4 hkl 1	$4\,m\,m$ 4 hkl 1
hk0	ditetragonal prism 8 m··	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 8 1	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 8 1	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 8 1	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 8 1	tetragonal prism 4 m··	$4\,/\,m$ 4 1	$4\,/\,m$ 4 1
100	tetragonal prism 4 mm2·	tetragonal prism 4 ·2·	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 4 ·m·	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 4 ·m·	tetragonal prism 4 ·2·	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 4 hk0 m··	$\bar{4}\,2\,m$ 4 1	$4\,2\,2$ 4 1
110	tetragonal prism 4 m·m2	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 4 ··m	tetragonal prism 4 ··2	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 4 ··m	tetragonal prism 4 ··2	$\frac{4}{m}\,\frac{2}{m}\,\frac{2}{m}$ 4 hk0 m··	$\bar{4}\,m\,2$ 4 1	$4\,2\,2$ 4 1
001	parallelo-hedron 2 4mm	parallelo-hedron 2 2·mm	parallelo-hedron 2 2mm·	monohedron 1 4mm	parallelo-hedron 2 4	parallelo-hedron 2 4	parallelo-hedron 2 2	monohedron 1 4

* A symmetry symbol in a pigeon-hole refers to the column where, in the same row, the name of the (limiting) form appears; the additional form symbol, for example {hkl} in pigeon-hole 4/m- {h0l}, is a reminder that here {h0l} is part of the general {hkl}. The dots in a face-symmetry oriented symbol stand for symmetry elements in the holohedry that are not part of the face symmetry; for example, in $\bar{4}m2$-{100}, face symmetry ·m· means that one of the two secondary mirrors is perpendicular to the face, both primary and tertiary elements being absent.

panying sheet (Table 2) provides, in the corresponding pigeon-hole of a similar double-entry table, the name of the form, its multiplicity and its face symmetry (that is, the symmetry elements normal to it) expressed in an oriented symbol[2]. The product of the multiplicity by the order of the face symmetry equals the order of the point group. The form names used (Table 1) follow the simplified nomenclature that evolved through the efforts of Groth, Rogers (1935), and Boldyrev (1936), followed by some missionary work by Donnay and Curien (1958) and Donnay and Takeda (1966).

The third lecture deals with periodicity in more detail. Both direct and reciprocal lattices are formally (and simultaneously) introduced by vector algebra, which our entering students have already been taught. The basic relation between reciprocal and direct lattice vectors is immediately accessible to them:

$$\mathbf{L}^*(hkl)\cdot\mathbf{L}(uvw) = (h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*)\cdot(u\mathbf{a} + v\mathbf{b} + w\mathbf{c})$$
$$= hu + kv + lw. \qquad (1)$$

If this scalar product is zero, the row $[uvw]$ lies in the net plane (hkl); whence (presto) $hu + kv + lw = 0$ is the famous "equation of zone control"! Likewise two rows $[u_1v_1w_1]$ and $[u_2v_2w_2]$ lie in net plane (hkl) if the vector product of two direct lattice vectors lies along the normal to (hkl), that is, if $\mathbf{L}(u_1v_1w_1) \times \mathbf{L}(u_2v_2w_2)$ is proportional to $\mathbf{L}^*(hkl)$ or if we have

$$h : k : l = \begin{vmatrix} v_1 & w_1 \\ v_2 & w_2 \end{vmatrix} : \begin{vmatrix} w_1 & u_1 \\ w_2 & u_2 \end{vmatrix} : \begin{vmatrix} u_1 & v_1 \\ u_2 & v_2 \end{vmatrix}.$$

The students already know the expression for the volume of the parallelepiped—$\mathbf{a} \times \mathbf{b} \cdot \mathbf{c}$; so much for the volume of the triclinic cell! From this formula the cell volume in every crystal system will be calculated in the laboratory.

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[2] The use of dots to orient symbols goes back to Patterson (1959) (p. 31, col. 1). This symbolism has been generalized and extensively used (Fischer *et al.*, 1973; Donnay and Turrell, 1974); it has been adopted, to designate site symmetry in space groups, in the forthcoming edition of *IT*.

The early laws of observation can now be taught in terms of either lattice, direct or reciprocal: (1) Faces grow $\parallel$ direct-lattice net planes (*hkl*) [or $\perp$ reciprocal-lattice vectors $\mathbf{L}^*(hkl)$], hence the Constancy of Angles (Romé de l'Isle, 1772; 1783). (2) Faces are $\parallel$ families of net planes with large $d(hkl)$ [or $\perp$ short $\mathbf{L}^*(hkl)$], hence the Simple Rational Indices (Haüy, 1784). (3) The larger the d [or the shorter the $\mathbf{L}^*$], the more frequent and the larger the corresponding face usually is; that is the Law of Bravais (1849–1850), amazingly successful as a first approximation at elucidating crystal morphology from lattice extinctions only. (The effect of space-group extinctions will come later.)

In the following lectures, the 32 point-group symmetries that are *possible in crystals* are derived by a combination of Gadolin's stereographic approach and some additional group theory. We first derive the 5 single rotation axes 1, 2, 4, 3, 6; then the four direct products with one 2-axis normal to the singular axis; finally the two cubic groups 23 and 432, thus reaching the total of 11 holoaxial groups. From them the remaining groups follow: 10 non-centrosymmetric ones as "mixed products", and 11 centrosymmetric ones (the Laue-Friedel classes) as direct products, with the center $\bar{1}$ (Donnay, 1967).

Two theorems are proved here: (1) a lattice has a center at any node, and (2) if a lattice has an n-axis with $n > 2$, it also has n 2-axes perpendicular to it. This information enables the class to pick, out of the 32 point groups left on the blackboard, the 7 symmetries *possible in lattices*. These lattice symmetries form the basis of the classification into our 7 crystal systems. Such a system embraces all the crystals that possess the same lattice symmetry; the symmetry of the crystal itself is either the same as, or lower than, the symmetry of the lattice—the two cases are referred to as the holohedry and one of the merohedries, respectively. (These are old concepts, once reviled, now revived.) For examples of merohedries, take point group 3: as 31, it is the tetartohedry of $\bar{3}2/m$ (rhombohedral lattice) and, as 311, the ogdohedry of $6/m2/m2/m$ (hexagonal lattice). The students are warned that this classification, which goes back to Mallard (1879) if not to Bravais (1849), and was admirably presented by C. Hermann in *IT* (1935, p. 54–60), is unfortunately no longer used in later Tables (Henry and Lonsdale, 1952); these adopt a division based on a purely formal criterion: any axis 6 or $\bar{6}$ (as long as it is not called $3/m$!) makes the crystal hexagonal; a singular 3 or $\bar{3}$, on the other hand, brands it as "trigonal." A so-called "trigonal system" is thus erected, in disregard of the primordial importance of the lattice symmetry. As a homework assignment the students are asked to emulate the *IT* and split the cubic system into two systems, according as the point-group symmetry of the crystal begins with a 4 or a $\bar{4}$, or with a 2 or a $2/m$. This exercise shows them the triviality of the *IT* criterion that splits our 12 hexagonal point groups into 7 hexagonal classes and 5 trigonal classes. A "trigonal" crystal should be placed in the rhombohedral system if its lattice is rhombohedral, into the hexagonal system if its lattice is hexagonal (Donnay, 1977).

The last two lectures before midterm are devoted to the lattice relations that govern twinning according to observations (Friedel, 1926) and the classification of twins (Friedel, 1926; Donnay and Donnay, 1974). In the meantime, in the laboratory, the students have learned how to use the Wulff net, in plotting the stereographic projection of chalcanthite, for which they have been given a full set of goniometric data taken from the literature. They have measured synthetic chalcanthite crystals on the two-circle goniometer. They have also spent part of one afternoon identifying the plane groups of two Escher drawings (MacGillavry, 1965), so as to familiarize themselves with glide reflections and the problem of choosing an origin. In class, glide planes, screw axes, and finally space groups are introduced in sufficient detail to enable the students to find their way through *IT*, volume I (1969). In the laboratory, crystal data for chalcopyrite are provided, and the students are instructed to draw the crystal structure in plan and elevation. A ball-and-stick model of the structure is placed at their disposal. This very popular assignment insures their understanding of the role space groups and point-positions play in structural crystallography.

The second part of the course: structural (X-ray) crystallography

X-ray crystallography is launched with the derivation of the Laue conditions for diffraction. We remind the student of the condition for a one-dimensional diffraction grating (that he studied in Optics) to give constructive interference,

$$(\mathbf{s} - \mathbf{s}_0)\cdot\mathbf{a} = h\lambda \qquad \text{or} \qquad (1/\lambda)(\mathbf{s} - \mathbf{s}_0)\cdot\mathbf{a} = h,$$

where a is the spacing of the grating, $\mathbf{s}$ and $\mathbf{s}_0$ are unit vectors directed along diffracted and incident beams, and h is *any* integer. The same relation applies to the $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ repeat vectors in a crystal, which at this point is just a lattice of diffracting points. The *random* integers are called h, k, l. The three equations are multiplied by x, y, z, respectively, these three quantities being *any* real numbers; *e.g.*, the trimetric coordinates of a point in the cell. The equations are then added; they give

$$(1/\lambda)(\mathbf{s} - \mathbf{s}_0)\cdot(x\mathbf{a} + y\mathbf{b} + z\mathbf{c}) = hx + ky + lz \quad (2)$$

or

$$(1/\lambda)(\mathbf{s} - \mathbf{s}_0)\cdot\mathbf{r}(xyz) = \mathbf{L}^*(hkl)\cdot\mathbf{r}(xyz) \quad (3)$$

in which the RHS of equation (2) is interpreted in the light of equation (1). The single Laue condition

$$(1/\lambda)(\mathbf{s} - \mathbf{s}_0) = \mathbf{L}^*(hkl) \quad (4)$$

results, *not* because $\mathbf{r}(xyz)$ can be "cancelled" from both sides of equation (3), but because the position vector $\mathbf{r}(xyz)$ stands for *any* vector, so that the only way equation (3) can be satisfied for more than one $\mathbf{r}$ vector is for the first vector in the dot products to be one and the same vector, as expressed by condition (4). This proof is one of the trickiest points to put across in the whole course. It is not difficult, on the other hand, to make the students independently rediscover Ewald's construction as the geometric expression of condition (4); for young students this is an exhilarating feat, in view of the elegance of the results, which they will not soon forget. From Ewald's construction they also derive Bragg's law on inspection (another kudo!):

$$\sin\theta = (\mathbf{L}^*(hkl)/2)/(1/\lambda) \text{ or } 2d(hkl)\sin\theta = \lambda. \quad (5)$$

Here we point out that the h, k, l were introduced into equation (4) as *any* integers. If coprime, they are Miller indices of a "reflecting" plane; if not, their common factor is n, the order of the reflection—the confusing n that students now thoroughly understand and can henceforth serenely omit, as in equation (5). The class is now ready to understand the geometry of *all* the experimental diffraction procedures, for single crystal and powder alike.

In the laboratory, to bridge the gap between morphological and structural crystallographies, we begin with the precession method. The students receive their copies of two zero-level films, $(001)^*_0$ and $(010)^*_0$, and a c cone-axis film of chalcanthite. They are shown how to identify the Laue class and crystal system. They then index the reflections on inspection, after they have been shown the positive directions of a^*, b^*, and c^* on the zero-level films. They measure the films on home-built light-boxes equipped with ruler and vernier that permit reading to ±0.05mm; for angular measurements they use the standard precession film readers. They obtain values for a^*, b^*, c^*, β^*, and γ^*. Knowing the recorded dial settings at which the two axial reciprocal-lattice nets were irradiated, they find the angle α through which the crystal has been rotated and, using a relation given in Appendix *a*,

$$\cos\alpha^* = \cos\beta^*\cos\gamma^* - \sin\beta^*\sin\gamma^*\cos\alpha,$$

they compute α^*. They are now ready to plot the edges of the reciprocal-lattice cell on a stereographic projection by means of the Wulff net and to find, on the same projection, the edges of the direct-lattice cell. By comparing this plot with the one previously obtained from morphological data, they draw conclusions as to relative accuracies: the goniometric data are good to a few minutes of arc; the film measurements are accurate to ±0.3 percent (lengths) and ±5′ (angles) at best. All but one of the interfacial angles they had previously been given are also measurable on the two films. The identity between interfacial angles, measured on the goniometer, and interrow angles, measured on precession films, is well understood by now. So is the usefulness of the reciprocal lattice for morphological as well as structural studies.

The cone-axis film is measured to obtain the c repeat, which is compared with the c value calculated from the reciprocal-lattice cell dimensions. A computing form, dating back to pre-computer days, once used for refining the cell dimensions of triclinic alkali feldspars from powder data (Donnay and Donnay, 1952, Table 3, p. 120) is included in the Manual; it permits checking, by hand, each step in the calculation from reciprocal to direct triclinic cell or *vice versa*.

The last and most time-consuming laboratory assignment deals with powder patterns. The students may bring their own unknown or they are given a cubic phase, which they X-ray in Debye-Scherrer (or Gandolfi) cameras. They measure the film, correct for shrinkage with the help of sharp shadow steps appearing every 10°0′ on the film, and convert the measurements to d values by using appropriate Tables (Fang and Bloss, 1966). They use L^* ($=1/d$) values to index the lines of the cubic patterns. For tetragonal or hexagonal samples, indexing charts are provided; for lower symmetries, no indexing is required. The more ambitious students are given mixtures of high-symmetry phases, but of different grain sizes, and so learn about "chemical fractionation by diffraction." Actual determination is carried out from strong lines by means of the *Powder Data File*, and from the axial ratios by means of *Crystal Data* (Donnay and Ondik, 1973).

The lectures are now turning to the weighted reciprocal lattice, whose importance in Laue-class determination has been realized in the laboratory. The displacement x, corresponding to phase angle φ in simple harmonic motion (SHM) with amplitude A, can be written $x = \mathrm{A}e^{i\varphi}$ (Appendix *e*). X-rays propagate with SHM and, if they are scattered by one electron at the origin, say, and another at a point x, y, z in the cell, we derive (Fig. 1)

$$\varphi/2\pi = \delta/d(hkl) = \delta\ |\mathbf{L}^*(hkl)| \tag{6}$$

and (omitting the hkl)

$$\delta = \mathbf{r}\cdot\mathbf{u}, \text{ with } \mathbf{u} = \mathbf{L}^*/|\mathbf{L}^*|, \text{ so that } \delta = \mathbf{r}\cdot\mathbf{L}^*/|\mathbf{L}^*|.$$

Substituting δ into equation (6), we obtain a phase angle φ_j for the j^{th} atom

$$\varphi_j = 2\pi\{\mathbf{r}(x_jy_jz_j)\cdot\mathbf{L}^*(hkl)\} = 2\pi(hx_j + ky_j + lz_j).$$

With scattering factor f_j the contribution of the j^{th} atom to the amplitude of the scattered wave is thus $f_je^{i\varphi_j}$. The sum of the contributions of all N atoms in the cell is the structure factor

$$F(hkl) = \sum_{j=1}^{N} f_{j,\theta}\, e^{2\pi i(hx_j+ky_j+lz_j)}\, e^{-B_j(\sin\theta)/\lambda} \tag{7}$$

The isotropic temperature factor B is explained qualitatively, as are anisotropic factors, so that the student will know what these parameters mean when he runs across them in a structure paper.

The structure factor exists in the complex plane and can be written as the sum of its real and imaginary parts (Appendix *d*):

$$\begin{aligned} F_{hkl} &= A_{hkl} + iB_{hkl} \\ &= f_j\left[\sum_j \cos 2\pi(hx_j + ky_j + lz_j)\right. \\ &\quad \left. + i\sum_j \sin 2\pi\,(hx_j + ky_j + lz_j)\right], \end{aligned} \tag{8}$$

where the summations are taken from $j = 1$ to $j = \mathrm{N}$. It is seen that the phase angle $\varphi = \arctan B/A$. For centrosymmetric crystals the student derives a phase angle of 0 or 180° and structure factors that are real. He must satisfy himself that the systematic extinctions he has derived geometrically for morphology can also be derived analytically here by substituting coordinates of symmetry-related atoms into the structure-factor expression.

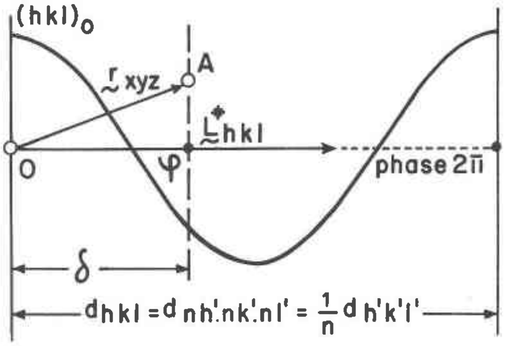

Fig. 1. Calculation of $F(hkl)$. The interplanar distance is $d(hkl)$, where h, k, l may contain a common factor n, so that it corresponds to a phase difference of 2π. The phase φ of an atom at point (xyz) is to 2π as δ is to d.

The concept of the electron-density function $\rho(xyz)$ is presented as the Fourier transform of weighted reciprocal space:

$$\rho(xyz) = \sum_h \sum_k \sum_l F_{hkl}\, e^{-2\pi i(hx+ky+lz)} \tag{9}$$

There is no time to go into details of Fourier summations or least-squares refinements, but the old Patterson-Tunell strips (1942) are shown in class to demonstrate the calculation of a one-dimensional Fourier series.

The final lecture

The final lecture tells of some exciting recent development in the field of mineralogical crystallography. This year the class learned of an "absolute" electron-density determination carried out on low-quartz by R. F. Stewart, of Carnegie-Mellon University (private communication). It shows the Si–O bond to be 75 percent covalent and only 25 percent ionic; the 50/50 description of the past 50 years, which was based on the electronegativity difference between Si and O, is incorrect.

The emphasis at the end of the course is placed on the fact that mineralogical crystallography is very much alive and going places! Anybody who tries to tell you otherwise has lost touch with reality.

Acknowledgments

The *Ministère de l'Education* of the Province of Quebec has generously defrayed the cost of the first printing of the *Crystallographic Laboratory Manual.* We thank Professor J. S. Stevenson, McGill University, for a critical reading of the manuscript.

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Manuscript received, February 21, 1978, accepted for publication, April 25, 1978.