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William Lawrence Bragg

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William Lawrence Bragg: The Pioneer of X-ray Crystallography and His Pervasive Influence

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Bragg, William Lawrence · crystallography · history of chemistry · Laue, Max · X-ray diffraction

A hundred years ago, a series of events that took place in the universities of Munich, Würzburg, Leeds, and Cambridge gave birth to one of the most important scientific developments of the 20th century. These events shed light not only on the way scientists of that era worked, they also illumine the sociological and emotional factors that often impel creative scientists. The protagonist of this story, William Lawrence Bragg, graduated with high honors in mathematics, but his approach to science was an artistic, imaginative one. In the words of one of the acolytes he influenced most, Max Perutz, "*he thought visually rather than mathematically generally in terms of concrete models … His artistic gifts surfaced in his delicate sketches and water colours, and in his limpid prose.*"[39]

1. 1912 and Laue's Spectacular Breakthrough and Bragg's Seminal Paper

Although 1913 marks the year when X-ray crystallography, through the determination of the structures of sodium chloride, potassium chloride, potassium bromide and potassium iodide[1,2] and of diamond,[3] first made its striking impact, two crucial, related events occurred in 1912. The first took place in May of that year when Max Laue, Walter Friedrich, and Paul Knipping submitted a paper[4] to the Bayerische Akademie der Wissenschaften in Munich that contained experimental proof that X-rays were waves not corpuscles, thereby settling a controversy that had lasted seventeen years since Röntgen's discovery.

The second occurred in the autumn of 1912 when William Lawrence Bragg (henceforth WLB), then a 22-year-old graduate student had an idea,[5] while walking along the Backs of Cambridge that "led immediately", in the words of his Royal Society biographer, Sir David Phillips,[6] "to a dramatic advance in physics" and has since transformed chemistry, mineralogy, metallurgy, and, most recently, biology. He realized that the observations of X-ray diffraction by a crystal, which had been reported by Laue and his associates earlier in the year,[4] can be interpreted very simply as arising from reflection of the X-rays by planes of atoms in the crystal and hence that the X-ray observations provide evidence from which the arrangement of atoms in the crystal may be determined. A few weeks of intensive work on simple inorganic compounds were enough to demonstrate the correctness of these ideas but the development of the method, at first in association with his father (William Henry Bragg, henceforth WHB) and later as the leader or guiding influence of a host of workers, was the "labor of a lifetime".

When WLB passed away in July 1971, X-ray crystallography had revealed the arrangement of atoms in matter of all kinds—and much more (see Section 5)—from the simplest salts and minerals to the macromolecules, including enzymes, and the genetic components of the living cell.

To date, about two dozen Nobel Prizes can be related in one way or another to X-ray crystallography. The series begins in 1914 with the Nobel Prize in Physics for von Laue[7] "*for the diffraction of X-rays on crystals*", followed by that for the Braggs (father and son) in 1915 and ends with the 2009 Prize in Chemistry for V. Ramakrishnan, T. A. Seitz, and A. E. Yonath for their "*studies of the structure and function of the ribosome*"[8] and D. Shechtman's prize in 2011 for the structure of quasicrystals. At present, X-ray crystallography is arguably the single most powerful analytical tool at the disposal of the physical, biological, materials, medical, and earth scientist and many breeds of engineer. It is still at the cutting edge of these sciences and has its fruitful impact also on mathematical aspects of crystallography (see Figure 1).

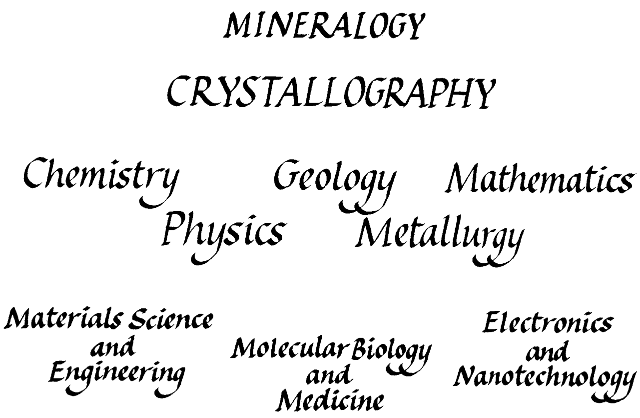

Figure 1. X-ray crystallography plays a central role in structural investigations in many scientific fields; reproduced with kind permission from Professor Moreton Moore.

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2. How Did the Braggs Become Acquainted with Laue's Discovery?

"It is not quite clear", so wrote[9] Paul Ewald, a physicist of major significance in Munich at the time of the Laue–Friedrich–Knipping work and for a long time afterwards,[8] "how the news of Laue's discovery reached England, and, in particular, W. H. Bragg". Laue himself thought that it was through the off-prints of the Academy papers which he sent out very soon to all those whom he considered to be immediately interested.[10] In July 1912, the Royal Society celebrated in London its 250th anniversary, and among the representatives from Germany was W. Voigt of Göttingen. He must have known of Laue's work through E. Madelung and through the talk that A. Sommerfeld had given to the Physical Society of Göttingen not long after 8 June (the date at which Sommerfeld communicated to the Bavarian Academy of Sciences the Laue–Friedrich–Knipping paper). According to Ewald[9] it would only be natural that Voigt spoke of it to his British colleagues, especially J. J. Thomson. But it is now known with certainty from the WHB archives[11] in the Royal Institution of Great Britain that Lars Vegard,[12] a Norwegian physicist (who later became famous for his work on auroral phenomena and the electronic structure of atoms), was the person who gave WHB all the facts. In 1912, Vegard was working with W. Wien in Würzburg, where he attended a lecture given there by Laue, who described in detail the results of the diffraction experiment (Vegard's letter to WHB on 26 June 1912 is reproduced in full in Ref. [12]).

Laue's idea was truly revolutionary. As he himself related[13] much later "*many people irradiated crystals with X-rays before Friedrich and Knipping. However, their observations were limited to the directly transmitted ray, which revealed nothing remarkable beyond the weakening produced by the crystal: they missed completely the less strong diffracted rays. It was the theory of the space lattice*[14] *which provoked the idea of investigating the neighbourhood of the direct ray*". As others[13] have opined, that is what makes the difference between idea-driven research and an accidental discovery.

Figure 2 shows an X-ray photograph of the mineral zinc blende, one of the eleven "Laue diagrams" contained in the Laue–Friedrich–Knipping paper of 1912;[15] it demonstrates the existence of internal atomic regularity in crystals and its relationships to the external symmetry of the mineral. Whilst this paper is a major landmark in X-ray physics and in the science of crystallography, revealing, as it did, ways of recovering quantitative information about the internal structure of crystalline solids, it yielded a relatively complicated way of evaluating the separation distances between atoms. Laue and his co-workers envisaged crystals in terms of a three-dimensional network of rows of atoms and based their analysis on the notion that a crystal behaves, in effect, as a three-dimensional grating. W. L. Bragg's picture, which we discuss below (Figure 3), was to regard a crystal as composed of layers or sheets of atoms which behaved in effect as reflecting planes, for which the angle of incidence equals the angle of reflection, strong "reflected" (i.e. diffracted) beams being generated when the path difference between reflections from successive planes in a family is equal to an integral number of wavelengths. This idea gave rise to the extremely simple, well-known Bragg equation[16] (also known as Bragg's Law; Eq. (1))

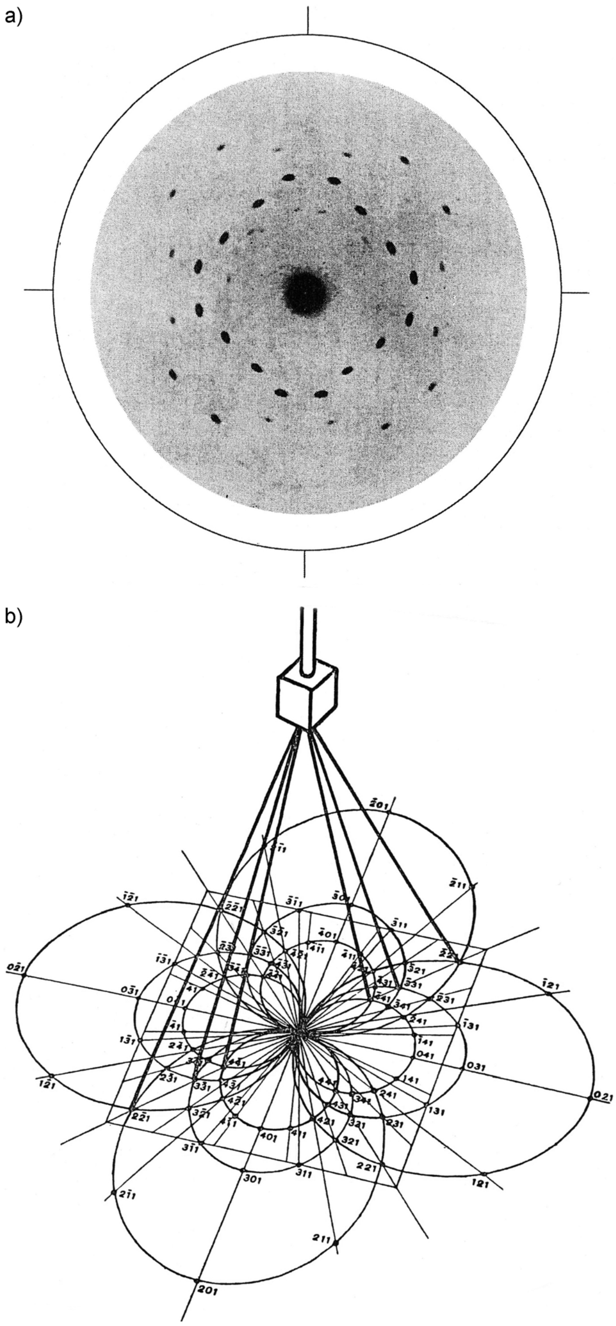
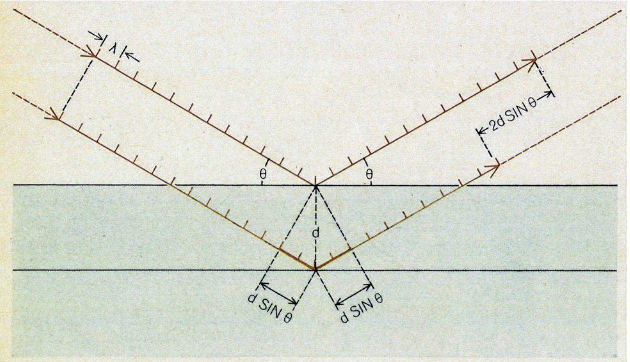


Figure 2. a) The X-ray photograph of zinc blende (ZnS) published by Friedrich, Knipping, and Laue in 1912.[4a] b) Drawing showing the mode of formation of a Laue X-ray photograph; reproduced from W. H. Bragg, *An Introduction to Crystal Analysis*, Bell and Sons, London, **1928**.

$$n\lambda = 2\,d\sin\theta \qquad (1)$$

where λ is the wavelength of the incident X-rays, n is the order of the reflection, d is the interplaner spacing, and θ is the angle of incidence to the planes.



BRAGG'S LAW, first formulated by the author in 1912, states the condition for diffraction of an incident beam of monochromatic X rays by the successive sheets of atoms in a crystal. In general terms the law states that if the path difference for waves reflected by successive sheets of atoms is a whole number of wavelengths, the wave trains will combine to produce a strong reflected beam. In more formal geometric terms, if the spacing between the reflecting planes of atoms is d and the glancing angle of the incident X-ray beam is θ, the path difference for waves reflected by successive planes is $2d \sin\theta$. In this diagram the extra path followed by the lower ray (*heavy colored line at bottom*) is four wavelengths long, which is exactly equal to the path difference of $2d \sin\theta$ between the two diffracted rays (*upper right*).

Figure 3. W. L. Bragg's interpretation of how diffraction of X-rays arises from reflection at atomic planes; reproduced from Ref. [31].

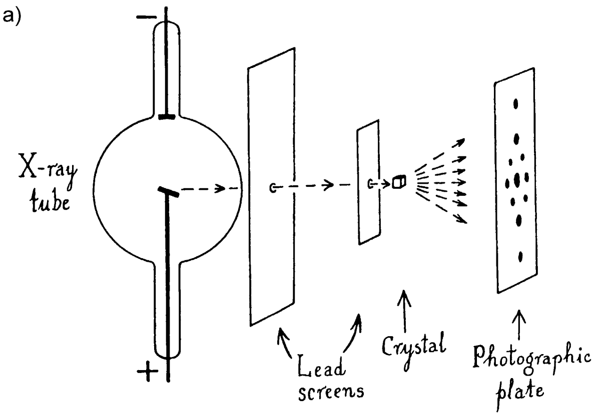
3. The Essence of WLB's 1912 and 1913 Papers

Even before WLB published, in his own name, his monumental 1913 paper[1] on the "Structure of some crystals as indicated by their diffraction of X-rays", and the one with his father on the structure of diamond,[3] he had presented to the Cambridge Philosophical Society on 11 November 1912 his seminal contribution entitled[16] "On the diffraction of short electromagnetic waves by a crystal".[17] This change in terminology arose because, during the summer of 1912 he had discussions with his father—then Professor of Physics at the University of Leeds—the possibility of explaining Laue's patterns by some other assumption than that of diffraction of waves. WLB convinced himself that the phenomenon described by Laue et al. was diffraction right enough, but he also convinced himself that Laue's analysis of the way it took place was not correct.

To appreciate readily the essence of WLB's improvement on Laue's interpretation we show in Figure 4 both a general view of the Laue setup, and the key interpretive diagram in WLB's assessment of the nature of Laue diagrams, such as that shown in Figure 2.

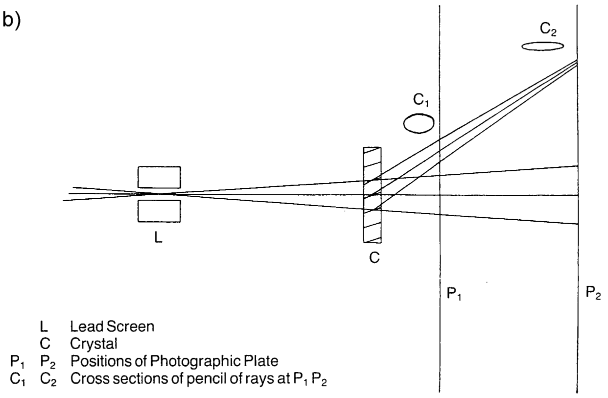
In WLB's own words[2] "*when the plate was placed at P_1, near the crystal the spots were almost circular like C_1, but when placed farther back at P_2 they became very elliptical (C_2). Now Laue had ascribed his pattern to the diffraction of certain specific wavelengths in the X-ray beam by the regular pattern of the crystal. Given a fixed wavelength, optical theory tells us that the diffraction must take place at a definite angle, and this means that the diffracted rays drawn in the picture should all have been parallel. I worked out that such pulses of no definite wavelength should not be diffracted only in certain directions, but should be* reflected *at any angles of incidence of the sheets of atoms in the crystal as if these sheets were mirrors*". In the setup depicted in Figure 4b (taken from WLB's paper of 1912, the rays are drawn as if reflected, and moreover, they close together again vertically while continuing to spread horizontally, thus explaining why the spots get more elliptical as the plate is placed farther away (note the ellipticity of the spots in Laue's photograph in Figure 2).

a)



Laue's experiment.

b)



Change of shape of the X-ray reflexions as the photographic plate was moved away from the crystal. Reflexions that were round when the plate was near the crystal became drawn out in the horizontal direction further away. Bragg pointed out that reflexion by the lattice planes of an incident cone of X-rays of continuously varying wavelength would come to a focus in the vertical direction, but would spread out in the horizontal direction

Figure 4. a) General view of the setup for the production of a Laue X-ray photograph. b) The diagram published by W. L. Bragg in 1912 that led him to propose reflection from atomic planes as the essence of X-ray diffraction; reproduced from Ref. [16].

Continuing WLB's commentary[16] on his 1912 paper: "*It remained to explain why certain of these atomic mirrors in the zinc blende crystal reflected more powerfully than others, a difficulty which had led Laue to postulate a group of definite wavelengths*" in his X-ray source. WLB showed that if the structure of ZnS is of the cubic-close-packing type, where the atoms are at the vertices at the center of the cube faces—and not only at the vertices (which was the assumption made by Laue et al.)—then he could explain why certain of the atomic mirrors in the ZnS crystal reflected more powerfully than others. He could also account for "absences" in the spot patterns.

WLB worked with feverish intensity (with his father) in the summer of 1912,[18] and, inter alia repeated the work of Laue et al. The importance of this Cambridge Philosophical Society paper for the further development of the field of X-ray crystallography to which Laue had found the access, can "hardly be overestimated", according to Ewald.[9] It contains three major points:

1) The idea of explaining the Laue spots as *reflections* of the incident ray on the internal net-planes;
2) The assumption of a continuous spectrum (i.e. "white" X-rays) of the incident ray and the *selective action* of the sets of reflecting planes in reenforcing only those wavelengths which fit into their distances of repeat;[19] and
3) The proof that the lattice for ZnS is not the simple cubic one (envisaged by Laue), but a face-centered cubic lattice.

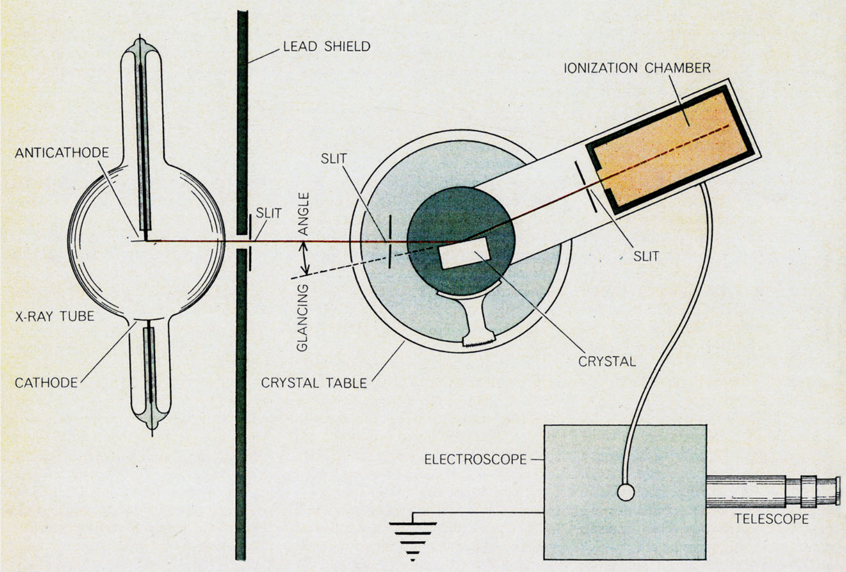


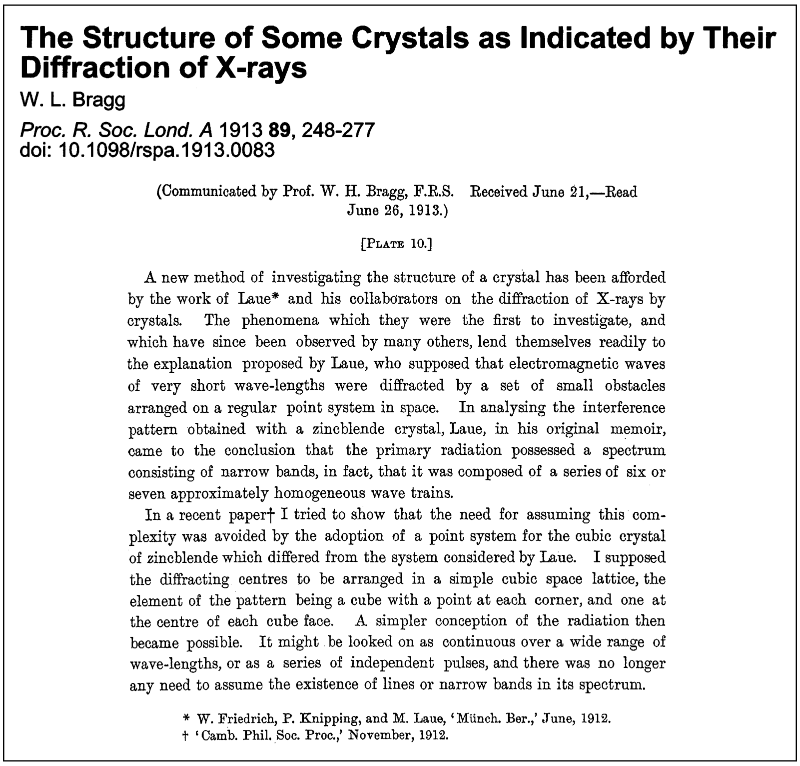
Figure 5. W. L. Bragg's depiction of the so-called X-ray spectrometer designed by his father, W. H. Bragg; reproduced from Ref. [31].

The concept of internal reflection does not contradict Laue's concept of diffraction, rather it is only a different form of expressing the same results, but it is far simpler to visualize. Ewald, as early as 1915,[9] following his introduction of the important concept of reciprocal lattice, showed that Laue's method and Bragg's method of determining crystal structures are essentially equivalent. It was in his 1912 paper that the famous Bragg equation first appeared, although it was cast in the less familiar form $n\lambda = 2d\cos\theta$, where, in this case, θ is the angle of incidence against the normal to the plane. Whereas Bragg's equation is well known, few people are aware of Bragg's second law that encapsulates a human attribute associated with WLB (see Section 9).

In the discussion following WLB's paper in Cambridge, 11 November 1912, C. T. R. Wilson[20] suggested that if the internal planes reflected, external crystal faces might also reflect as well, provided their roughness was small enough. WLB quickly carried out such a reflection experiment using mica, well-known for its perfect cleavage faces—and, true enough, after allowing an X-ray beam to graze such a surface at approximately 10°, Bragg saw the specularly reflected beam on his photographic plate.

The first scientist to be stimulated by WLB's brilliant studies was his father, WHB, who made certain that the reflected rays could be detected in an ionization chamber as well as photographically. This experiment must have been the conclusive stimulus for WHB's construction of the so-called X-ray spectrometer (Figure 5), the instrument which for decades was to be the main tool for crystal structure analysis throughout the UK and in many other countries.

WLB made use of his father's X-ray spectrometer, as well as his own assembled Laue setup, while still a graduate student at the Cavendish Laboratory, from where he published his pioneering paper,[1] the opening paragraphs of which, in view of their historical importance and elegant clarity are shown in Figure 6. In this paper he reports both Laue photographs and X-ray spectrometer traces—more correctly diffractometric traces—of the minerals sylvine (KCl), rock salt (NaCl), zinc blende (ZnS), fluorspar (CaF_2), calcite ($CaCO_3$), and iron pyrites (FeS_2).



The Structure of Some Crystals as Indicated by Their Diffraction of X-rays

W. L. Bragg

Proc. R. Soc. Lond. A 1913 **89**, 248-277
doi: 10.1098/rspa.1913.0083

(Communicated by Prof. W. H. Bragg, F.R.S. Received June 21,—Read June 26, 1913.)

[Plate 10.]

A new method of investigating the structure of a crystal has been afforded by the work of Laue* and his collaborators on the diffraction of X-rays by crystals. The phenomena which they were the first to investigate, and which have since been observed by many others, lend themselves readily to the explanation proposed by Laue, who supposed that electromagnetic waves of very short wave-lengths were diffracted by a set of small obstacles arranged on a regular point system in space. In analysing the interference pattern obtained with a zincblende crystal, Laue, in his original memoir, came to the conclusion that the primary radiation possessed a spectrum consisting of narrow bands, in fact, that it was composed of a series of six or seven approximately homogeneous wave trains.

In a recent paper† I tried to show that the need for assuming this complexity was avoided by the adoption of a point system for the cubic crystal of zincblende which differed from the system considered by Laue. I supposed the diffracting centres to be arranged in a simple cubic space lattice, the element of the pattern being a cube with a point at each corner, and one at the centre of each cube face. A simpler conception of the radiation then became possible. It might be looked on as continuous over a wide range of wave-lengths, or as a series of independent pulses, and there was no longer any need to assume the existence of lines or narrow bands in its spectrum.

* W. Friedrich, P. Knipping, and M. Laue, 'Münch. Ber.,' June, 1912.
† 'Camb. Phil. Soc. Proc.,' November, 1912.

Figure 6. The opening paragraphs of WLB's seminal paper; reproduced from Ref. [1].

The analysis of these crystal structures by WLB "*was initially undertaken with the object of discovering the absolute wavelength in centimetres of the homogeneous radiations issuing from the X-ray bulb. The position on the curves (of the 'spectrometer') gave the wave-length of the corresponding radiation in terms of the dimensions of the crystal space lattice. As long as the complexity of the unit associated with each point of the lattice is unknown, the absolute wavelength cannot be calculated. If the arrangement here assigned to the alkaline halides is right, the dimensions of the lattice can be given in centimetres, for the mass associated with each centre of the lattice can be calculated from the known mass in grammes of the hydrogen atom*". WLB continues[1] that for rock salt the mass of one molecule of NaCl is $58.5\times 1.64\times 10^{-24}$ g, hence:

$$58.5\times 1.64\times 10^{-24} = V_p = 33.3\times 2.15\,\lambda^3 \qquad (2)$$

$$\lambda^3 = 1.34\times 10^{-24}\ \text{cm}^3,\ \lambda = 1.10\times 10^{-8}\ \text{cm} \qquad (3)$$

From the value of λ, and that for d/λ given in Table X of WLB's paper,[1] the dimensions of the lattice of any crystal in that table can be calculated. To be sure, in order to determine the X-ray wavelength it is necessary to know Avogadro's number and the density of the crystal.

4. WLB's Personal Thoughts on His and WHB's Breakthrough

At the first conference on X-ray Analysis in Industry (held under the auspices of the Institute of Physics) in 1942,[2] WLB gave an address from which the following remarks are taken:

"*The X-ray spectrometer opened up a new world. It proved to be a far more powerful method of analyzing crystal structure than the photographs which I had used. One could examine the various faces of a crystal in succession, and by noting the angles at which and the intensity with which they reflected the X-rays, one could deduce the way in which the atoms were arranged in sheets parallel to these faces. The intersections of these sheets pinned down the positions of the atoms in space. On the other hand, a suitable crystal face could be used to determine the wave-lengths of the characteristic X-rays coming from different elements as sources. It was like discovering an alluvial gold field with nuggets lying around waiting to be picked up. At this stage my father and I joined forces and we worked furiously all through the summer of 1913, using the X-ray spectrometer. Although the description of this instrument was published in our joint names, I had no share in its design. The capital I brought to the family firm was my conception of reflection and the application in general of the optical principles of diffraction, and my success in analysing the first crystals by the Laue method. It was a glorious time, when we worked far into every night with new worlds unfolding before us in the silent laboratory. My father was at first far more interested in X-rays than in crystals, and left the determination of crystal structure to me, with the exception of a paper on diamond which showed the power of the instrument he had devised. He measured the wave-lengths of the X-ray spectra given by the elements platinum, osmium, iridium, palladium, rhodium, copper and nickel. He identified them with Barkla's K and L radiations. He calculated their energy quanta according to Planck's relationship, and showed that this agreed with the energy of the cathode rays required to excite them. He showed that the shortest wave-lengths (Kα and Kβ) from various elements were similar, and that they were approximately inversely proportional to the square of the atomic weight. This was in fact a first hint of the subsequent brilliant generalization of this principle by Moseley,*[21] *who used it to determine the atomic numbers. In fact, he laid the firm foundations of X-ray spectroscopy, afterwards to be so brilliantly developed by Moseley and Siegbahn.*[22] *I remained true to my first love, the determination of crystal structure. By using measurements on crystals made with the X-ray spectrometer, many of them due to my father, I was able to solve the structures of fluor spar, cuprite, zinc blende, iron pyrites, sodium nitrate and the calcite group of minerals. I had already solved KCl and NaCl. These results were produced in a year (1913) of concentrated work, for the war in 1914 put an end to research*".

5. A Brief Résumé of Subsequent Developments

Both shock and exhilaration greeted the publication of the two 1913 papers of WLB and WHB. Shock, because it was incontrovertibly established that there was no molecule of sodium chloride inside rock salt, simply an extended alternation of sodium and chloride ions. Exhilaration, because the structure of diamond confirmed the tetrahedral coordination of carbon as envisaged by van't Hoff and others 40 years earlier.

From 1913 onwards two distinct methods became available by which X-rays could be used to elucidate the details of crystal structure. In the Laue method, polychromatic X-rays penetrate the crystal and gave rise to a spot pattern on a photographic plate or film. In the Bragg method, monochromatic X-rays are reflected from a set of parallel planes. Because the results were more readily translated into structural information by means of the intensity of the diffraction lines, and also because the Braggs (WHB especially) were dextrous in the use of ionization detectors, the Bragg method was usually preferred over the Laue one for several decades. Some workers, notably Linus Pauling, used X-ray Laue photographs and (so-called) X-ray spectrometer readings to determine crystal structures (see, for example, the Pauling group work on hematite (Fe_2O_3) and corundum (Al_2O_3),[23] barite ($BaSO_4$),[24] brookite (TiO_2),[25] topaz ($Al_2SiO_4F_2$),[26] and micas[27]).

Since the principal purpose of this Essay is to celebrate the centenary of the 1913 work of WLB and also to highlight what led to his winning the Nobel Prize in Physics 1915[28] (Figure 7), only a short outline is given of the major developments in X-ray crystallography that occurred subsequently. These have, in any case, been chronicled in unequal detail (up to 1962) in Ewald's classic text,[9] in a charming piece by WLB himself[29] (in 1960) published in *Science*, in a *Nature* article[30] marking the 80th year of the WLB breakthrough, and in

Figure 7. William Lawrence Bragg in 1915, the year he was awarded the Nobel Prize in Physics; photograph kindly provided by his son, Dr. Stephen Bragg.

a beautifully lucid semipopular article in *Scientific American*[31] composed by WLB (see below).

In an article entitled "Architecture of the Invisible" I summarized[30] the principal achievements of X-ray crystallography up until 1993; and in the January 2012 issue of *Acta Crystallographica*, D. Schwarzenbach recalls[32] the success story of crystal structure determination by X-ray diffraction, in which the impact of computers and the creation of data banks as well as the study of disordered structures and thermal motion are adumbrated.

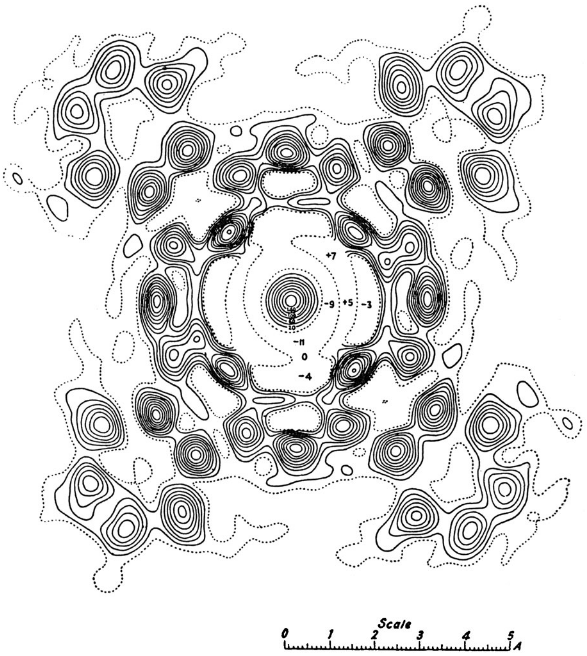
Once it became almost routine, a dozen years or so ago, for investigators to gain access to high-flux synchrotrons,[33] the Laue method again began to be extensively employed, especially for charting time-resolved structural changes at sub-picosecond and femtosecond resolutions.[34] It was speculated[35] in 2009 that, with the availability of free-electron lasers (and their enormous fluxes), such as that in operation at Stanford, that the required "crystal" size of specimens may shrink all the way down to single molecules; three-dimensional movies of conformational dynamics and chemical processes would be possible as well as the imaging of macromolecules that cannot be readily crystallized. J. H. C. Spence and colleagues[36] have introduced a novel approach, designated serial femtosecond crystallography (SFX), to X-ray structure determination in which femtosecond (synchrotron) pulses impinge upon a stream of droplets containing biologically significant macromolecules. In a paper published[36] exactly 100 years to the month since the revolutionary advances followingthe work of Laue et al. in Bavaria, the X-ray free-electron laser (XFEL) consortium of 19 groups has convincingly demonstrated, with SFX, that it is no longer necessary to cool crystals to cryogenic temperatures (as is conventional in normal X-ray crystallography) to minimize the radiation damage inflicted on the sample by the high flux of X-rays, which is the usual case in other synchrotron studies. Instead, using ultrashort pulses (ca. 70 fs) one capitalizes on the providentially convenient principle of "diffract-then-destroy". This method uses X-ray pulses that are sufficiently intense to produce high-quality diffraction which are of short enough duration to terminate before the onset of substantial radiation damage and the destruction of the sample. (X-ray pulses of only 70 fs duration terminate before any chemical damage and the destruction of the sample processes can occur.)

The limpid clarity of the *Scientific American* article,[31] which WLB wrote when he was 78 years old, constitutes a model summary of all the main techniques and resolved problems (up to that time) of X-ray crystallography—rotation and Weissenberg photographs, powder diffraction, the heavy-atom method, the determination of X-ray phases and stereochemical configurations, and order–disorder phenomena. He also gives a beautiful analysis of his father's far-reaching idea, proposed[37] in 1915, that the periodic repeat of atomic patterns in crystals could be represented by Fourier series: "*If we know the nature of the periodic variation of the density of the medium we can analyze it by Fourier's method into series of harmonic terms..We may even conceive the possibility of discovering from the [relative X-ray] intensities the actual distribution of the scattering centres, electrons and nucleus of the atom*." Undoubtedly, this advance by WHB was stimulated by Ewald's work in introducing the concept of the reciprocal lattice.[9]

The Fourier method, which WLB described as the "complete reversal" of his earlier own method of solving crystal structures became a standard technique even in the mid-1930s. Indeed, J. M. Robertson's Fourier transform representation of the electron-density distribution in a molecule of platinum phthalocyanine (Figure 8) became a popular exemplar of the new method. Once it was shown (by Bennett and Kendrew)[38] how digital, programmable computers could be readily used to compute Fourier syntheses, the processing of diffraction data consisting of hundreds of thousands of measured X-ray diffraction intensities could be and have been undertaken by the agency of ever-more powerful computers.

WLB's synoptic article in *Scientific American*[31] also recalls many other key advances that X-ray crystallography has uncovered. Handsome homage is paid by him to his rival Linus Pauling, and, in particular, to the enunciation of Pauling's rules and the brilliant manner in which, from Pauling and WLB's work on silicates, the enormous variety of distinct structures exhibited by silicates were united by Pauling into one syncretistic whole. This article also highlights the vitally important work of Debye, not only in demonstrating the importance of temperature in influencing X-ray intensities, but also (with Scherrer) in introducing the widely used Debye–Scherrer method of X-ray diffractometry for the analysis of powder samples. He also alludes to the dramatic advance contained in Dorothy Hodgkin's work on the crystal analysis of vitamin B_{12}. Her discovery that a cobalt enzyme (vitamin B_{12}) contains an adenosyl group linked to cobalt by a direct Co−C σ bond was, therefore, rather surprising. Her work also revealed a structural motif, the so-called corrinoid ligand system, not previously encountered in natural product chemistry.

WLB also noted how the DNA structure yielded its secrets through X-ray data acquired from fibrous materials, a sensational advance not only because it disclosed a compelling mechanism for the process of heredity, but also vast ramifications in the entire corpus of molecular biology and genetics. In reference to Perutz's brilliant discovery that



An electron density map showing the structure of the molecule of platinum phthalocyanine. The peak at the center (the platinum atom) is really very much higher than any of the others.

Figure 8. The electron density contours of platinum phthalocyanine produced from observed X-ray diffraction intensities using the method of Fourier syntheses. In this early representation (taken by J. M. Robertson in the late 1930s) it is not possible to detect the hydrogen atoms. (Present-day methods utilize computer programs that directly reveal the atomic positions at the nodes shown here in the contour maps.) Reproduced from J. M. Robertson, *Organic Crystals and Molecules*, Cornell University Press, **1953**.

certain heavy atoms such as Hg, I, or Au could be chemically attached to specific points of macromolecules like the globular proteins without disturbing the crystal structure—a discovery that led, in turn to the determination of the molecular structure of both myoglobin and hemoglobin—WLB made the remark, so characteristic of his mastery of analogy, that complex macromolecules take no more notice of the isomorphous attachment of a heavy atom than "*a maharajah's elephant would of the gold star painted on its forehead*".[31]

WLB concluded his *Scientific American* article by citing the landmark achievement of his colleague, David C. Phillips, in the Royal Institution determination of the (first-ever) structure of the enzyme lysozyme. Not only did this enzyme exhibit β-sheets and α-helices, the occurrence of which was predicted by Pauling, but it also afforded convincing proof of the mode of chemical action of the enzyme itself.

A measure of WLB's perspicacity is disclosed in the final paragraph of his *Science* paper of 1960.[29] In pondering the quest for the determination of molecular structure he asks "*Why is this so important?*" He answers, "*The function of these molecules must be dependent upon their geometry. They must fit each other in just such a way that the right parts are brought into conjunction and can interact chemically. We hope to understand such processes when we know the structure; we hope to see how the enzymes act, why vitamins are necessary, what hormones do, why certain substances are poisonous*".

He composed these words 45 years after winning the Nobel Prize. As others have testified (see Section 6), WLB was imbued by an unquenchable scientific curiosity.

6. WLB's Qualities and Achievements as Perceived by His Contemporaries and Co-Workers

The opinions of three of his colleagues who all won Nobel Prizes in 1962, as well as the views of a few others who worked alongside him illustrate the essence of WLB the man, and his approach to science. According to Max Perutz:[39]

"*Bragg united C. P. Snow's two cultures because his approach to science was an artistic, imaginative one. He thought visually rather than mathematically generally in terms of concrete models that can be either static, like his crystal structures, or dynamic … like mobile dislocations in metals. His artistic gifts surfaced in his delicate sketches and water colours, and in his limpid prose*" (see Figure 9).

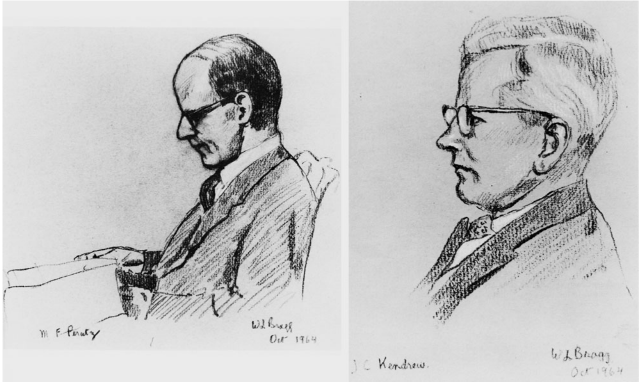


Figure 9. Max Perutz (left) and John Kendrew (right) as portrayed by WLB; reproduced from Ref. [39].

Perutz's co-recipient of the 1962 Nobel Prize in Chemistry, Sir John Kendrew, said[40] of WLB that:

"*Basically he was a puzzle-solver; to him the great fascination was to interpret the complicated diffraction pattern, say of a protein crystal, in terms of its three-dimensional structure … Bragg was one of the last of the classical physicists, who never involved himself much with the ideas of quantum theory or of particle physics*".

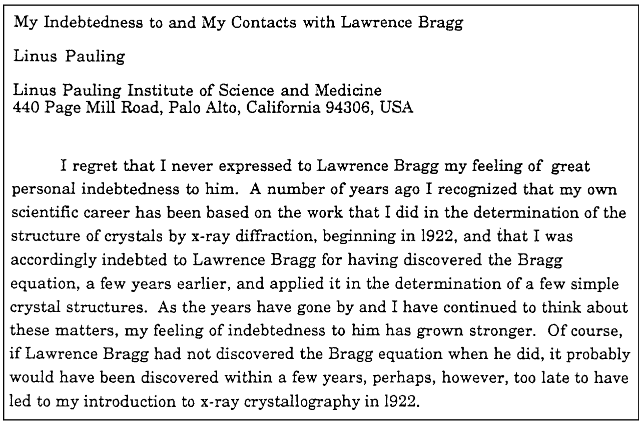
Francis Crick recalls:[41]

"*I did not meet Bragg till I was about 33. I was much in awe of him. As the founder of X-ray crystallography, he was already a legendary figure. He obtained his Nobel Prize for his pioneer work in the year before I was born. As Head of the Cavendish, he held the senior physicist chair in Britain. He was, in addition, the boss of my supervisor, Max Perutz (I had yet to obtain a Ph.D),*[42] *and took a keen and largely constant interest in Perutz and Kendrew's attempts to solve the thee-dimensional structure of a protein.*

"*Thanks to Jim Watson's chatty account*[43] *of our experiences at the Cavendish between 1951 and 1953, it is public knowledge that Bragg did not always find my company entirely agreeable. He felt I was too critical, partly because of my detailed comments on the current work in the group, but mainly because I had argued, at a fairly public meeting, that most of their efforts stood little chance of succeeding. 'Crick,' he said to me, 'you're rocking the boat.'*

"*He also thought I talked too much and, I suspect, in too fast and complicated a manner, often about scientific subjects that he probably felt had little to do with X-ray crystallography. Nevertheless, I learned a lot from Bragg. He was a major influence on my scientific career. Perhaps the most useful and lasting lesson was how to approach a scientific problem. One example will explain what I mean. I had been trying to deduce mainly from Perutz's data, the approximate overall shape of the haemoglobin molecule. I started off in the right way, but I got bogged down in details. Also, I did not look around for other evidence. Bragg quite independently took up the problem, made some bold simplifying assumptions, was not too pernickety about the exact fit with the experimental data as I had been and, with Perutz, came up with a good first approximation to the shape that fitted several distinct unit cells. It was a lesson I have never forgotten*".

Writing to me in May 1990, from his Institute of Science and Medicine in Palo Alto, California, Linus Pauling expressed the views shown in Figure 10.[44]



My Indebtedness to and My Contacts with Lawrence Bragg

Linus Pauling

Linus Pauling Institute of Science and Medicine
440 Page Mill Road, Palo Alto, California 94306, USA

I regret that I never expressed to Lawrence Bragg my feeling of great personal indebtedness to him. A number of years ago I recognized that my own scientific career has been based on the work that I did in the determination of the structure of crystals by x-ray diffraction, beginning in 1922, and that I was accordingly indebted to Lawrence Bragg for having discovered the Bragg equation, a few years earlier, and applied it in the determination of a few simple crystal structures. As the years have gone by and I have continued to think about these matters, my feeling of indebtedness to him has grown stronger. Of course, if Lawrence Bragg had not discovered the Bragg equation when he did, it probably would have been discovered within a few years, perhaps, however, too late to have led to my introduction to x-ray crystallography in 1922.

Figure 10. First paragraph of a typescript received by the author from Linus Pauling, June 1990.

Pauling also went on to say that he, his wife, and oldest son, Linus, Jr., had spent a month with WLB in Manchester in the spring 1930, when he was much welcomed and helped by the Bragg family. Nevertheless, Pauling[45] was disappointed with his stay there largely because

"*Bragg did not ever ask me to discuss scientific matters with him, and I, his junior by eleven years, did not have courage enough to ask for such a discussion with him or to suggest that I might give a seminar … I had determined the structures of some silicate minerals, as had also Bragg and his co-workers … In the spring of 1948, when I was Eastman Professor at Oxford, we visited Cambridge and were graciously received by Bragg and Lady Bragg … At that time, too, Bragg and I did not have any serious discussions about science, whereas every time that I came in contact with Bernal we were at once engaged in a lively interchange of ideas. Some years later I was told that Bragg resented my having intruded into the fields of crystallography and mineralogy in which he was working, and that he considered me to be a competitor … Without having much supporting evidence, I surmise that circumstances during the second half of the 1920s may have influenced Bragg's life. At that time, although still quite young, he held an important position in science, involving administrative and teaching duties, as well as the direction of research. As a result, when quantum mechanics was discovered he was not in a position to devote enough time to this rather complicated and somewhat abstruse subject to master it. I suggest that he may have felt handicapped by this lack, and that it may have kept him from entering into lively scientific arguments and discussions.*"

The reflections of three other crystallographers, all of whom worked alongside him, merit inclusion. H. S. Lipson[46] said:

"*I claim that W. L. Bragg is the most successful scientist in history. I accept that Newton and Einstein have greater reputations, but although all three did their greatest work in their early twenties, Newton and Einstein essentially spent the rest of their lives polishing up their ideas. Bragg went on for the whole of his life transforming different branches of science. He first of all revolutionized chemistry, then mineralogy, then metallurgy and finally biology.*"

Lord Phillips of Ellesmere (D. C. Phillips), who along with his then PhD student Louise Johnson revealed the precise mode of operation of lysozyme—the first ever enzyme to have its structure determined (under WLB's aegis at the Royal Institution[47])—said:[6]

"*Bragg was certainly one of the great creative scientists yet he often worried about his relative lack of more mundane gifts. Forgetful of names, uneasy on committees, reluctant to face personal problems or angry scenes, he depended a great deal on his wife who sustained him through all the triumphs and difficulties of a long public life.*"

Jack Dunitz,[48] the doyen of present day X-ray crystallographers, wrote in 1990:

"*In my life I have met many great scientific figures of the twentieth century. In the multi-dimensional space describing the various qualities, gifts and talents, any comparison becomes impossible. Sir Lawrence Bragg stands out among them through the simplicity and directness of his physical intuition, and for something else: he was one of the last of a disappearing variety of human being—he was a gentleman.*"

7. Research and the Popularization of Science at the Royal Institution

WLB resigned his Cavendish Chair in Cambridge in 1953 to take up the post of Director and Fullerian Professor in the Royal Institution of Great Britain and the Directorship of the Davy-Faraday Research Laboratory (DFRL) there. He set about assembling a new research team at the DFRL devoted to protein crystallography. He wanted both Max Perutz and

John Kendrew to move with him from Cambridge to London. They refused to do so, but agreed to come to the DFRL on an approximately one day per week basis as Honorary Readers, posts that they each held for some 13 years, until WLB was succeeded by George Porter. This was an admirable compromise, as it harmonized with WLB's other action, namely the appointment of Dr. David C. Phillips, whom he attracted to the DFRL from Canada. (Phillips had earlier gained an initial degree in Physics, Mathematics and Electrical Communications at the University College of South Wales, Cardiff before completing a PhD under the supervision of the eminent crystallographer A. J. C. Wilson). Uli Arndt, German-born but educated at Cambridge, joined the DFRL at the same time; others followed, like J. D. Dunitz from Glasgow, Caltech, and Oxford and Tony North from King's College, London.

With encouragement from WLB, Phillips and Arndt built a linear automatic X-ray diffractometer, the first in the world. This instrument, adapted to make multiple simultaneous measurements of diffraction intensity, was to have profound consequences. With this diffractometer, Phillips and his team, including his PhD student Louise Johnson were able to achieve data of high accuracy that led in turn to precise protein structures. The instrument was first used[47] to extend the data of the myoglobin crystals to 1.4 Å resolution, a remarkable achievement. Myoglobin, solved first by John Kendrew,[49] became the first protein to have its structure determined in atomic detail. It was work of Nobel Prize winning significance.

Phillips' work on lysozyme[47,50] started at the DFRL in 1961. The solution of its X-ray structure was achieved in 1965, in time for the dual celebration of Bragg's 75th birthday and the 50th anniversary of his Nobel Prize. The structure showed the complete path of the polypeptide chain (of 129 amino acid residues) folded into both α-helices, which had previously been identified in myoglobin, and β-sheets, a feature that had been predicted by Linus Pauling but had not hitherto been observed in three dimensions. Phillips' work under WLB's aegis was of enormous significance biologically: it contributed to knowledge on protein folding (still a topic of major interest); it clearly revealed the existence of a catalytically active site consisting of aspartic acid (at position 52) and glutamic acid, which, at position 35, is in a hydrophobic pocket. This work constituted the first time that structure had provided an explanation of how an enzyme catalyzed a chemical reaction.[47]

George Porter has given[51] a fascinating account of how WLB took him into the so-called Model Room in the basement of the Royal Institution, one night in 1965. On the table in the middle of the room, illuminated by one electric bulb, was an imbricated pile of perspex sheets, on each of which had been drawn the electron density cross sections of a very large molecule. It was lysozyme. This achievement by Phillips and his team brought WLB to the brink of ecstasy.

Whereas WLB was primarily concerned on the research front in fostering the application of X-ray crystallography to biological problems, while at the Royal Institution he also wrote, with the Director of Mineralogy at the British Museum (Natural History), C. F. Claringbull, *Crystal Structures of Minerals*.[52] This became and remains to this day an invaluable *vade mecum* for mineralogists and solid-state chemists.

At the Royal Institution, WLB also put enormous effort into attracting speakers for the program of Friday Evening Discourses, thereby continuing the tradition initiated by Michael Faraday.

As Max Perutz once wrote,[39] "*WLB's superb powers of combining simplicity with rigour, his enthusiasm, liveliness and charm and his beautiful demonstrations conspired to make him one of the best lecturers on science that ever lived.*"

Like his father WHB, who was also at the helm at the Royal Institution (from 1923 to 1942), and Faraday himself, WLB took his lecturing to a lay audience and to schoolchildren extremely seriously (Figure 11). His "*Advice to Lecturers*", is an anthology taken from the writings of Michael Faraday and Lawrence Bragg,[53] illustrates several of his aphorisms concerning how to deliver a memorable lecture. One excerpt from that publication will suffice:

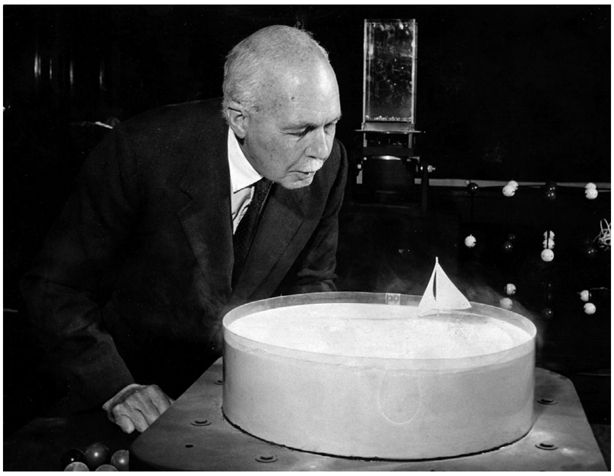


Figure 11. William Lawrence Bragg gave brilliant popular lectures. Here he demonstrates a toy boat sailing on a fluidized bed of sand; photograph kindly provided by Dr. Stephen Bragg.

"*A good lecture is a tour de force; a good lecturer should be keyed up to a high pitch of nervous tension before it and limp and exhausted after it … If a sensitive lecturer is to give of his best, he must be left in peace for a period before the lecture starts. It is the refinement of cruelty to expect him to be social, to introduce him to a number of people whom he has not met before and to whom he must be polite…*"

A favorite mantra recalled by WLB when talking about lecturing was also regularly used by the Italian-American physicist Enrio Fermi: "*Never underestimate the pleasure that people derive from hearing the things they already know.*" One of the gems in his (and Faraday's) advice to lecturers starts with the following words: "*A lecture is made or marred in the first ten minutes. This is the time to establish the foundations to remind the audience of things they half knew already and to define terms that will be used.*"

8. Biographical Sketch of WLB

WLB was born in Adelaide, South Australia in 1890. He enrolled at the University of Adelaide at age 15 and obtained a first class degree in mathematics before he sailed to England with his family in 1909 when his father, WHB, was appointed Head of Physics at the University of Leeds. He entered Trinity College, Cambridge, and achieved first class honours in Part I of the mathematics course, during which he attended lectures by G. H. Hardy and A. N. Whitehead. He switched to Natural Science for Part II of his course where he again registered high marks, graduating with a B.A. in 1912. He was appointed Fellow and Lecturer in Natural Sciences at Trinity College in 1914, and began his research in the Cavendish Laboratories under the supervision of J. J. Thomson. Of this period he later wrote in his unpublished autobiography in 1970 that:

"*…it was a sad place at that time. There were too many young researchers … too few ideas for them to work on, too little money, and too little apparatus. We had to make practically everything ourselves…we had to do our own glassblowing and there was only one foot-pump for the blow-pipe…J.J. set me on some problem on the variation of ionic mobility with the saturation of water vapour…but with my self-made crude set-up [the results] were meaningless…After a year of this, however, my golden opportunity came. Von Laue published his paper on the diffraction of X-rays by zinc blende and other crystals and my father discussed it with me when we were on holiday at Cloughton on the Yorkshire coast, staying with friends.*"

This was the summer holiday of 1912. The first break-through was made by WLB after he returned to Cambridge, when he noticed that the spots in Laue's photograph were elliptical in shape (see Figure 2a). The Braggs then worked with febrile intensity in 1913 as described above, and published their seminal work.

At the outbreak of the First World War, WLB enlisted with the Royal Artillery and was posted to France in August 1915, where he became an expert in "sound-ranging", the technique he developed to determine the location of enemy guns by recording the times it took for the sound to reach strategically placed detectors. WLB's personal life was deeply affected during the autumn of 1915 by the death of his brother Bob at Gallipoli, where Moseley was also killed.[54] News of a different kind, the award of 1915 Nobel Prize for Physics to him and his father, came when he was setting up the first sound-ranging station near the front line in Ypres. (The village priest with whom he was billeted produced a bottle of Lacryma Christi).

In 1919 WLB was appointed to succeed Ernest Rutherford at Manchester University, where he held the Langworthy Chair, arguably, at that time, the second most important in Britain after the Cambridge Chair, where Rutherford succeeded J. J. Thomson. In 1921 he was elected Fellow of the Royal Society and he also married. At Manchester he transformed our knowledge of both minerals and alloys, but Pauling was running neck and neck with him in the first of these ventures. WLB made splendid progress in solving the structure of quartz and numerous silicate minerals, including the exceptionally difficult task of elucidating the structure of diopside ($CaMg(SiO_3)_2$) with B. Warren.[55] He used Fourier series to determine the structure of many solids. And with E. J. Williams wrote a series of beautiful papers on order–disorder phenomena in alloys.[57] An excellent account of the many milestones reached by WLB in his Manchester days has been given by Helliwell.[58]

In 1937 WLB left Manchester to become Director of the National Physical Laboratory in Teddington, a move which he soon realized was taken more for social than scientific reasons. This appointment was short-lived. When Rutherford died in 1937 steps were taken in Cambridge to attract WLB, a decision that was not well received by the nuclear and particle physicists who were still working at the Cavendish Laboratory. But almost as soon as WLB took office the Second World War intervened, and WLB was principally involved in war work. However, he had taken note of and given much encouragement to the lonely and ostensibly rabbinically complicated endeavors of Max Perutz, who had come to Cambridge from Vienna to work with J. D. Bernal because, as he later proclaimed, he wanted to solve a great problem in biochemistry. Bragg's support of the work of Perutz and Kendrew led, in 1947 to the establishment of a Medical Research unit on the molecular structure of biological macromolecules. His support of Martin Ryle and Anthony Hewish's work in radioastronomy at the Cavendish Laboratory was also strong. (All four individuals in due course won Nobel Prizes.) But he experimented with optical analogues of X-ray diffraction, and, with his students J. F. Nye and W. M. Lomer,[59] devised "bubble rafts" on the surface of water to simulate dislocations, grain boundaries, and other features of crystalline defects. All the while, the Perutz–Kendrew group grew stronger and it attracted, amongst others, James Watson, Francis Crick, and Hugh Huxley.

Bragg resigned his Chair at Cambridge to take up responsibilities at the Royal Institution in 1953. Even after retirement as Director there in 1966 he composed many fine popular articles such as: "The Art of Talking about Science",[60] "The Spirit of Science",[61] and "What Makes a Scientist",[62] as well as his famous foreward to *The Double Helix* by Watson.[43] In it he said that Watson "*writes with a Pepys-like frankness. Those who figure in the book must read it in a very forgiving spirit.*"

In his career he published 257 papers and 13 books, many of which were translated into several languages, none more so than the write-up of his Royal InstitutionI Christmas Lectures entitled "*Electricity*" in 1936 which was also published in Swedish, 1937; Polish, 1939; Czech, 1940; Hungarian, 1948; Finnish, 1950; German, 1951; Japanese, 1951; and Italian, 1953.[63]

9. Bragg's Second Law

The uniqueness of Bragg's law of diffraction is so widely acknowledged that any suggestion that there exists a second law bearing the same eponym inevitably stimulates curiosity. During the final stages of the writing of this article, an old friend, Jack Dunitz, whose mythopoetical insights into the folklore of crystallography add an extra vitality to his conversation, suggested that I should tell the tale of Bragg's Second Law. Full details of the story were published by the prime witness of the enunciation of the "Second Law", the late E. W. Hughes (EWH),[64a] in a book entitled *Patterson and Pattersons* published by the International Union of Crystallography and Oxford University Press in 1987.[64b]

Each year, the Department of Chemistry, Cornell University, Ithaca, invites a world-famous scientist to present the so-called Baker Lectures. The aim of this extended series is to highlight important advances in aspects of science of vital interest to chemists. The invited speaker takes up residence as Visiting Professor for a semester or more in the Baker Laboratory of the university, and is normally provided with a dynamic young assistant from the research or junior teaching staff of the department.

In the late winter of 1933, WLB was the Baker Lecturer and EWH his assistant. One weekend WLB went to visit A. L. Patterson at the Massachusetts Institute of Technology, and there he learned, prior to publication, about the Patterson method.[65,66] EWH takes up the story:[64b]

"*He arrived back at Ithaca early on a very bad winter's day; it had sleeted all night, then frozen and snowed slightly and the streets were sheets of ice. He arrived at the laboratory safely by taxi and asked if I could deliver him to a local appointment. My Model A Ford had sat out all night in a nearby parking lot and would not start. I suggested that he get in and steer while I pushed it down a nearby hill. He objected that he was not familiar with American cars and insisted that I operate it while he pushed. Fortunately it started and we set off south on East Avenue. The University B&G trucks had spread ashes on the east side of our road, but not yet on our side.*

"*He then started enthusiastically to tell me about the Patterson method, which he pronounced to be the most important advance since his father, WHB, had introduced the use of the Fourier series. He used the fingers of one hand to represent atomic position vectors and those of the other hand to represent their differences, and I soon forgot about the ice. Until suddenly, approaching Central Avenue, I became aware of a red traffic light and a heavy truck rushing west on Central to make his green light. Ashes had been spread on both sides of Central. We skidded about badly but by pure good luck lurched to the left onto the ashes at the last instant and scrunched to a halt, well into the intersection. The truck managed to swerve and miss us by about a foot. Our light turned green and I continued, very cautiously. Through all this Bragg continued to wave his hands and lecture on Patterson's vectors, but to a deaf audience! When he had finished there was a brief pause and he suddenly said, 'I say! We skidded a bit back there, didn't we?' Later, in the security of his office I got a repeat of the Lecture.*

"*The following year I was in England with proofs for the figures in his Baker monograph. Once, when we were driving (in his car) to his office we passed the scene of a recent bad road accident, which reminded me of what could have happened in Ithaca. I asked him if he remembered the incident and when he said that indeed he did, I remarked upon how impressed I had been by his calm nonchalance in the face of very real danger. He then stated what I have come to call 'Bragg's Second Law'.*

"'*When travelling in a foreign country I make it a point of personal honour not to show fear, anger, or mirth, or surprise at any happening that does not seem to be unusual to the natives.*'

"'*And,' he added, 'you didn't seem to be frightened so I was jolly well determined not be frightened either*'."

EWH ended his personal reminiscence of WLB by saying that he considered his "Law" to be excellent advice and "*…have tried to follow it, but one thing is clear; on that winter morning in Ithaca he was not very good at estimating the reaction of the native*".[64b]

I am deeply grateful for the constructive help given to me by Christopher Hammond (Leeds), Jack Dunitz (Zurich), John Helliwell (Manchester), Moreton Moore (London), John Spence (Arizona), John Davies (Cambridge), Kenneth Harris (Cardiff), Louise Johnson (Oxford), and Stephen Bragg (Cambridge).

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[1] "The structure of some crystals as indicated by their diffraction of X-rays": W. L. Bragg, *Proc. R. Soc. London Ser. A* **1913**, *89*, 248.

[2] W. L. Bragg, Remarks made at the First Conference on X-ray Analysis in Industry, held in Cambridge in 1942. Reproduced in full in Ref. [9].

[3] "The structure of diamond": W. L. Bragg, W. H. Bragg, *Proc. R. Soc. London Ser. A* **1913**, *89*, 277.

[4] "Interferenzerscheinungen bei Röntgenstrahlen": a) W. Friedrich, P. Knipping, M. Laue, *Münch. Ber.* **1912**, 303; b) "Eine quantitative Prüfung der theorie für die Interferenzerscheinunge bei Röntgenstrahlen": M. Laue, *Münch. Ber.* **1912**, 36.

[5] a) Somewhere between St. John's College and the site of Darwin College. b) It is remarkable that Laue recalls in his autobiography the very time and place when the idea for a mathematical explanation of the spots in the photographs taken by Friedrich and Knipping "occurred to him". It was not far from his apartment at Bismarkstrasse 22 just in front of the house at Siegfriedstrasse 10 in Munich.

[6] "William Lawrence Bragg": D. C. Phillips, Biographical Memoirs of Fellows of the Royal Society, **1979**, *25*, 1.

[7] Laue felt that his two co-workers should have shared the Nobel Prize with him, and he distributed the money equally between the three.[8]

[8] "Laue centennial": W. W. Schmidt, W. Steurer, *Acta Crystallogr. Sect. A* **2012**, *68*, 1.

[9] *Fifty Years of X-ray Diffraction* (Ed.: P. P. Ewald), International Union of Crystallography, Utrecht, **1962**, Sections I and II in particular. See also "Paul Peter Ewald": H. A. Bethe, G. Hildebrandt, Biographical Memoirs of Fellows of the Royal Society, **1988**, *34*, 134, especially pp. 153–155.

[10] In the 19th century it was common practice for physical scientists—and possibly others—to distribute reprints of their important papers to others across the globe. Willard Gibbs, at Yale, for example, sent a copy of his famous work on the phase rule to James Clerk Maxwell in Cambridge.

[11] Royal Institution of Great Britain Archives: RI MS WHB 7A/3.

[12] a) J. Jenkin, *William and Lawrence Bragg, Father and Son: The Most Extraordinary Collaboration in Science*, Oxford University Press, Oxford, **2008**, p. 326; b) "L. Vegard, C. R. Bury, and the electronic interpretation of the Periodic Table": M. Davies, *Arch. Hist. Exact. Sci.* **1990**, *40*, 185.

[13] Quoted in Ref. [8].

[14] A fact drawn to Laue's attention by his junior, Ewald.

[15] See Ref. [4].

[16] "The diffraction of short electromagnetic waves by a crystal": W. L. Bragg, *Proc. Cambridge Philos. Soc.* **1912**, *17*, 43.

[17] WLB avoided using the word X-rays out of respect for his father, who was an ardent believer that X-rays were corpuscles not waves.

[18] WLB had been given one of the five X-ray spectrometers that were made in the workshops of the Department of Physics, University of Leeds, to take to Cambridge; see *"The Bragg Notebook: A Commentary and Interpretation"*. http://www.leeds.ac.uk/library/spcoll/bragg-notebook/ written by Dr. Christopher Hammond; see also C. Hammond, *The Basics of Crystallography and Diffraction*, 3rd ed., Oxford Science Publications, Oxford, **2009**.

[19] The words used by WLB in his paper[16] are: "*the crystal actually 'manufactures' the light of definite wavelength, much as, according to Schuster, a diffraction grating does. The difference in this case lies in the extremely short length of the waves*".

[20] C. T. R. Wilson (1869–1959), Nobel Laureate, discoverer of the "cloud chamber". It was said of him by his contemporaries *"…the most gentle and serene, and the most indifferent to prestige and honours."* WLB said that Wilson's undergraduate lectures on optics were outstanding.

[21] H. G. J. Moseley (1887–1915). To investigate the positive charge on atomic nuclei, he examined their element-characteristic X-ray spectra.

[22] K. M. G. Siegbahn (1886–1978), a pioneer of X-ray spectroscopy, for which he won the Nobel Prize in Physics in 1924.

[23] "The crystal structures of hematite and corundum": L. Pauling, S. B. Hendricks, *J. Am. Chem. Soc.* **1925**, *47*, 781.

[24] "The crystal structure of barite": L. Pauling, P. H. Emmett, *J. Am. Chem. Soc.* **1925**, *47*, 1026.

[25] "The crystal structure of brookite": L. Pauling, J. H. Sturdivant, *Z. Kristallogr.* **1928**, *68*, 239.

[26] "The crystal structure of topaz": L. Pauling, *Proc. Natl. Head. Sci. USA* **1928**, *14*, 603.

[27] "The structure of the micas and related minerals": L. Pauling, *Proc. Natl. Head. Sci. USA* **1930**, *16*, 123.

[28] The Braggs are the only parent–child pair in history to share a Nobel Prize, and WLB remains the youngest ever to win the Prize at age 25.

[29] "British achievements in X-ray crystallography": W. L. Bragg, *Science* **1960**, *131*, 1870.

[30] "The architecture of the invisible": J. M. Thomas, *Nature* **1993**, *364*, 478.

[31] "X-ray crystallography": W. L. Bragg, *Sci. Am.* **1968**, *219*, 58.

[32] "The success story of crystallography": D. Schwarzenbach, *Acta Crystallogr. Sect. A* **2012**, *68*, 57.

[33] "Multiplicity distribution of reflections in Laue diffraction": a) D. W. J. Cruickshank, J. R. Helliwell, K. Moffat, *Acta Crystallogr. Sect. A* **1987**, *43*, 656; "Laue crystallography: coming of age": b) Z. Ren, D. Bourgeois, J. R. Helliwell, K. Moffat, V. Srajer, B. L. Stoddard, *J. Synchrotron Radiat.* **1999**, *6*, 891.

[34] "The recording and analyses of synchrotron radiation X-ray Laue photographs": D. W. J. Cruickshank, J. R. Helliwell, L. N. Johnson, *Philos. Trans. R. Soc. London Ser. A* **1992**, *340*, 167.

[35] "Imaging with X-ray free-electron facilities": H. N. Chapman, *Nat. Mater.* **2009**, *8*, 299; see also on this theme R. Neutze, R. Wouts, D. van der Spoel, F. Wechert, J. Hajdu, *Nature* **2000**, *406*, 752.

[36] "High-resolution protein structure determination by serial femtosecond crystallography": S. Boutet, J. C. H. Spence et al., *Science* **2012**, *337*, 362.

[37] "Bakerian Lecture: X-rays and Crystal Structure": W. H. Bragg, *Philos. Trans. R. Soc. London Ser. A* **1915**, *215*, 253.

[38] "The computation of Fourier syntheses with a digital electronic calculating machine": J. M. Bennett, J. C. Kendrew, *Acta Crystallogr.* **1952**, *5*, 109.

[39] M. F. Perutz in *Selections and Reflections: The Legacy of Lawrence Bragg* (Eds.: J. M. Thomas, D. C. Phillips), Science Reviews Ltd, London, **1990**, p. 71.

[40] J. C. Kendrew in *Selections and Reflections: The Legacy of Lawrence Bragg* (Eds.: J. M. Thomas, D. C. Phillips), Science Reviews Ltd, London, **1990**, p. 88.

[41] F. C. H. Crick in *Selections and Reflections: The Legacy of Lawrence Bragg* (Eds.: J. M. Thomas, D. C. Phillips), Science Reviews Ltd, London, **1990**, p. 109.

[42] Francis Crick won his Nobel Prize before he graduated with a PhD.

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[45] L. Pauling in *Selections and Reflections: The Legacy of Lawrence Bragg* (Eds.: J. M. Thomas, D. C. Phillips), Science Reviews Ltd, London, **1990**, p. 86.

[46] H. S. Lipson in *Selections and Reflections: The Legacy of Lawrence Bragg* (Eds.: J. M. Thomas, D. C. Phillips), Science Reviews Ltd, London, **1990**, p. 100.

[47] "Structure of some crystalline lysozyme–inhibitor complexes determined by X-ray analysis": D. C. Phillips, L. N. Johnson, *Nature* **1965**, *206*, 986.

[48] J. Dunitz in *Selections and Reflections: The Legacy of Lawrence Bragg* (Eds.: J. M. Thomas, D. C. Phillips), Science Reviews Ltd, London, **1990**.

[49] "A three-dimensional model of the myoglobin molecule obtained by X-ray analysis": J. C. Kendrew, G. Bodo, H. M. Dintzis, R. G. Parrish, H. Wyckoff, D. C. Phillips, *Nature* **1958**, *180*, 662.

[50] "The early history of lysozyme": See L. N. Johnson, *Nat. Struct. Mol. Biol.* **1998**, *11*, 942; see obituary of L. N. Johnson in Nature, 25 October 2012.

[51] G. Porter in *Selections and Reflections: The Legacy of Lawrence Bragg* (Eds.: J. M. Thomas, D. C. Phillips), Science Reviews Ltd, London, **1990**, p. 126.

[52] W. L. Bragg, C.F. Claringbull, *Crystal Structures of Minerals,* (G. Bell & Sons, London, **1965**.

[53] Advice to lecturers by M. Faraday and Lawrence Bragg (an anthology). Royal Institution of Great Britain, **1974**.

[54] Bob wrote home (see Ref. [12]) *"We had an awful mix-up when we landed: the arrangements here seem perfectly scandalous…-someone ought to get the sack."* My own father was in the Gallipoli landing. He told me, so inept was the planning, that within a few hours of landing, a third of the men around him lay dead.

[55] "The structure of diopside, $CaMg(SiO_3)_2$": W. L. Bragg, B. Warren, *Z. Kristallogr.* **1928**, *69*, 168. In his autobiography, WLB says that the structure of diopside was a turning point in our ideas about silicate structures. It showed that the "SiO_3" which appears in the chemical formula does not represent SiO_3 acid groups but a string of SiO_4 groups joined by shared oxygen atoms. It was a crucial step in showing that silicon always occurs in a tetrahedron group of oxygen atoms. Although this is largely true it is not invariably the case. A new silicate mineral, stishovite, was discovered in 1962 where Si^{4+} atoms are in sixfold coordination.[56]

[56] "Identifying the coordination for silicon by magic-angle-spinning NMR: Stishovite and quartz": J. M. Thomas, J. M. Gonzalez-Calbet, C. A. Fyfe, G. C. Gobbi, M. F. Nicol, *Geophys. Res. Lett.* **1983**, *10*, 91.

[57] "The effect of thermal agitation on atomic arrangements in alloys": W. L. Bragg, E. J. Williams, *Proc. R. Soc. London Ser. A* **1934**, *145*, 699.

[58] “X-ray crystal structure analysis in Manchester from W. L. Bragg to the present day (2002)”: J. R. Helliwell, *Z. Kristallogr.* **2002**, *217*, 385.

[59] a) “Blowing bubbles with Bragg”: See W. M. Lomer in *Selections and Reflections: The Legacy of Lawrence Bragg* (Eds.: J. M. Thomas, D. C. Phillips), Science Reviews Ltd, London, **1990**, p. 115; b) “A dynamical model of crystal structure”: W. L. Bragg, J. F. Nye, *Proc. R. Soc. London Ser. A* **1947**, *190*, 474.

[60] “The art of talking about science”: W. L. Bragg, *Mar. Technol.* **1967**, *4*, 258.

[61] “The spirit of science”: W. L. Bragg, *Proc. R. Soc. Edinburgh Sect. A* **1967**, *67*, 303.

[62] “What makes a scientist”: W. L. Bragg, *Proc. R. Inst. G. B.* **1969**, *42*, 397.

[63] A more complete list is given in J. M. Thomas, “Picking winners: W. H. and W. L. Bragg at the Royal Institution”, *Notes and Records of R. Soc.* **2011**, *65*, 163.

[64] a) E. W. Hughes received his research training at the Baker Laboratory, Cornell University. Apart from assisting WLB in preparing for publication the *Atomic Structure of Minerals* (Ithaca, 1937), he also assisted another Baker Lecturer, Linus Pauling, in the production for press of *The Nature of the Chemical Bond* (Ithaca, 1939). His crystallographic achievements were considerable. He was the first to introduce, in 1941, the use of the “least squares” fitting of crystallographic data. In 1964 he and his graduate student W. N. Lipscomb, who later won the Nobel Prize, further pursued the method of least squares to crystal structure refinement. b) E. W. Hughes in *Patterson and Pattersons* (Eds.: J. P. Glusker, B. K. Patterson, M. Rossi), International Union of Crystallography and Oxford University Press, **1987**.

[65] The X-ray methods used by WLB to solve the structure of rock salt and diamond, and by others to solve graphite and hexachlorobenzene involved trial and error. A major step forward in the feasibility of determining crystal structures by X-ray methods was provided by A. L. Patterson.

[66] In essence, Patterson’s contribution was to show that from the intensities of the various diffractions it is possible to construct a “vector map” that gives the distances between pairs of atoms. We may describe a “vector map”, following Judson,[67] using the analogy of a party. Everyone has their shoes nailed to the floor and everyone wants to meet everyone else! The vectors are the directions each person has to turn to shake the hand of another guest and how far that person has to extend his or her arms. The strength of the handshake is analogous to the atomic numbers of the two atoms at the end of the guests at the party. It is as if the only information one possesses about the party is the distance and angle of the handshake of each person when he or she met everyone else. Equipped with this complicated knowledge, it should then be possible to find where everyone stood in the room relative to each other.

[67] H. F. Judson, *The Eighth Day of Creation: Makers of the Revolution in Biology*, Simon and Schuster, New York, **1979**.