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Foundations of Crystallography

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Laue centennial

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A century ago, on the evening of 4 May 1912, three men dropped an envelope into the letterbox of the building of the Bayerische Akademie der Wissenschaften in Munich. They knew that the gentle thud was to be followed by a larger reverberation. They had hit two scientific jackpots. The envelope contained a preliminary report on an experiment which Max von Laue had suggested and Walter Friedrich and Paul Knipping had carried out in the weeks before. Their report held the experimental proof that X-rays were waves, which settled a controversy which had lasted 17 years since Röntgen's discovery; and at the same time it contained the proof that crystals, which they had just used successfully as a diffraction grating for X-rays, have a lattice-like structure on the molecular scale. Yet still, at that moment, the three men may not have been aware that their experiment was indeed the stepping stone for a giant leap for mankind – it would open the way to exploring the structure and chemical bonding of matter up to the understanding of the molecular basis of life. 'This step,' wrote Max von Laue later in his autobiography, 'which consisted essentially in the investigation of individual crystal structures was one I could hardly have taken myself. I have always been primarily interested in the great underlying principles in physics ... The Braggs, father as well as son, had a love for the individual substance and could devote their labour to the structure of crystals'

It took almost a century from the determination of the prototypic structure of NaCl to that of the ribosome, from the first Laue diffraction photographs with exposure times of hours to those of time-resolved X-ray crystallography with exposure times on the picosecond scale. So far, about two dozen Nobel prizes can be related in one or another way to crystallography. This impressive series starts in 1914 with the Nobel Prize in Physics for Max von Laue for the 'diffraction of X-rays on crystals,' followed rapidly by that for the Braggs in 1915, and it ends for the time being with the 2011 Nobel Prize in Chemistry for Dan Shechtman for the 'discovery of quasicrystals,' just two years after the Nobel Prize in Chemistry for V. Ramakrishnan, T. A. Steitz and A. E. Yonath for their 'studies of the structure and function of the ribosome.' 100 years after Laue, Friedrich and Knipping, crystallography is still at the cutting edge of science – from biology to engineering materials. The 50-year anniversary in 1962 was marked by four Nobel prizes: those for chemistry, physics, medicine and peace were awarded to scientists in the fields of condensed matter and molecular structure research. It gives an impression of Max von Laue's personality that he said publicly that it would have been more just to award his Nobel Prize to Friedrich and Knipping as well. Consequently, he shared the prize money with them. In 1923, Walter Friedrich became Professor for Medical Physics at the University of Berlin and in 1951 he became President of the German Academy of Sciences in Berlin (East). Paul Karl Moritz Knipping established an Institute for X-ray Physics at the University of Darmstadt in 1928, only with the title of Professor at that time; later he was promoted to a permanent position as Associate Professor. In 1935, while riding his motorcycle, he died in a road accident. Max von Laue returned to Berlin in 1919 and in 1922 became Deputy Director of the Kaiser-Wilhelm-Institut für

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Physik at the side of Albert Einstein as the Director. During the Nazi regime, Laue stood up for Albert Einstein and modern physics, and opposed the ideologic movement of the so-called 'Deutsche Physik'. In 1943 he was retired early. After the end of Nazi rule, Laue was one of the leading figures in the rebuilding and reorganization of physics in post-war Germany. In 1951 he became Director of the Fritz-Haber-Institute of the Max-Planck Society in Berlin-Dahlem. On 24 April 1960 Laue died in a car crash in Berlin, as he rushed from the Max-Planck-Institute to the new Hahn-Meitner-Institute research reactor, which owed its existence much to Laue's initiative and diplomacy.

Laue's fame for solid-state research with and without neutrons lived on in the name of the Institut Laue–Langevin, Grenoble, founded in 1967.

It is difficult to imagine the time when the periodic lattice of atoms or molecules in crystals was still a mysterious hypothesis, and when even the nature of X-rays was subject to speculations and controversial among the eminent scientists of the time. Before the Laue experiment, did anyone dream of tools allowing one to explore the structure of matter on the molecular scale and use this information for deriving structureproperty relationships of materials - or for understanding the molecular basis of life? After X-rays had already been used to image in vivo the internal anatomy of the human body, with the Laue experiment the internal structure of crystals also became accessible on the nanoscale. The poor quality of the first X-ray photograph taken by Friedrich and Knipping could have led to a misinterpretation as well, as a kind of absorption image like those taken on all kinds of materials earlier. As pointed out by Max von Laue in his autobiography: '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 which provoked the idea of investigating the neighbourhood of the direct ray.' This is what makes the difference between idea-driven research and an accidental discovery.

We wonder what would have happened if the theoretician Max von Laue had not met P. P. Ewald, who informed him that crystals were thought to have lattice periodicity, and if he would afterwards not have been able to convince experimentalists to perform the experiment ... who else would have done it, and when, for William Henry Bragg supported the particle nature

of X-rays at the time (the dualism of wave and particle was not realized until the thesis of Louis de Broglie, submitted in 1924).

Why are we publishing a joint issue of Acta Crystallographica Section A and Zeitschrift für Kristallographie on the occasion of Laue's centennial? One obvious reason is that both journals serve the crystallographic community and promote crystallographic research. Another reason is that the then Zeitschrift für Krystallographie und Mineralogie was the only journal at the time of Laue's discovery dedicated mainly to crystallography. Furthermore, Max von Laue was Editor of Zeitschrift für Kristallographie from 1924 to its discontinuation in 1945. The first issue of Acta Crystallographica, the newly established journal of the International Union of Crystallography (IUCr), appeared in March 1948, one year after the IUCr was founded with Sir Lawrence Bragg as the first President of the Executive Committee and Max von Laue as Honorary President. The publication of Zeitschrift für Kristallographie was not resumed until 1955.

The article by Henk Kubbinga, Crystallography from Haüy to Laue: controversies on the molecular and atomistic nature of solids, mainly focuses on the development of crystallography in the 19th century: how lattice and symmetry theory evolved from the observations available at the time. Michael Eckert illustrates in his critical essay Disputed discovery: the beginnings of X-ray diffraction in crystals in 1912 and its repercussions the scientific environment in which the Laue experiment took place. André Authier reviews in his article Optical properties of X-rays - dynamical diffraction the development of diffraction theory, while Dieter Schwarzenbach's contribution *The success story of crystallography* covers the history of structure analysis. A fifth paper, Multigrain crystallography by Sørensen et al., is published in the special issue of Zeitschrift für Kristallographie only, as a further contribution from the speakers at the Laue symposium that is to take place in March 2012 in Munich, Germany.

Although crystallography is today recognized as a mature science and crystal-structure analysis is still seen at its core, crystallography must not be reduced to its set of powerful diffraction techniques and methods. Crystallography is the interdisciplinary science that studies condensed matter of any origin from the structural point of view. Despite the fact that most scientists using crystallographic techniques would not call themselves crystallographers, the structural point of view has become crucial in all fields where structure–property or structure–function relationships play a role.