PETER GOODMAN 1928-1999

On March 26th 1999 one of the pioneering scientists in the field of electron diffraction, Peter Goodman, passed away in Melbourne, Australia. Peter had a long-term heart problem and though recently his health had been failing he was still active in research and supervising students. He is survived by his lifelong partner, Pat and their three children David, Robin and Richard, and five grandchildren. We have collected here contributions from many of Peter's colleagues which illuminate aspects of his outlook and achievements from a variety of perspectives, and we hope this mosaic reveals something of his character.

It is no exaggeration to say that the work he, Alex Moodie and Gunter Lehmpfuhl undertook established an entire field of science, which has since been taken up by many groups around the world. Peter performed world-class work on electron diffraction and his very careful and thorough work set extremely high standards for all other scientists involved in electron diffraction and microscopy. He published a number of absolutely seminal papers in the field.

Peter was a dedicated experimental physicist - and as such the most unassuming character that many had the pleasure of meeting. It seems that a thoughtful curiosity triggered him, in his experimental work in the lab, as in his highly innovative approach to some basic problems in the field of electron crystallography. His main and lasting contribution was the revival and development of convergent-beam electron diffraction (CBED) into a crystallographic tool. Recent crystallographic studies by convergent beam electron diffraction originated from Goodman and Lehmpfuhl (1965), although earlier work by Kossel and Möllenstedt (1939) was done about five decades ago. As Jon Gjønnes recalls Peter talked about this during his one-year stay in Oslo in the early 1960's. In that period he made several visits to Fritz-Haber-Institut in Berlin. He was interested in intensity measurement in electron diffraction, and had become critical of the way single crystal intensities were recorded by spot patterns ('cross-grating' patterns, as they were called). He explained that intensity profiles ('rocking curves') would be a more well-defined option - and proposed to use a convergent beam, focussed on the specimen. Such a probe-forming facility, which is standard in modern electron microscopes, was not available at that time. But Peter found, characteristically, an unconventional practical solution. Working with Gunter Lehmpfuhl at Fritz-Haber he placed a thin crystal in the objective aperture position, that is in the back-focal plane of a strong lens of a Siemens Elmiskop I. They obtained CBED patterns by converging a conical electron beam of an angle

of more than 10^{-3} rad on a small area of a specimen (~300Å) which had a uniform thickness and no bending. The CBED-patterns they obtained in this way marked the beginning of systematic application of this technique to determination of crystal symmetry, and structure factor refinement. Using a specimen goniometer of Peter's design, they first performed the determination of low-order crystal structure factors. This was the beginning of the modern CBED method. The low-order structure factor determination has been extensively studied especially by Drs. Zuo and Spence. Peter, who gave the real scientific value to the CBED method, was the true pioneer of the method. The story illustrates two sides of Peter's way of doing science: looking for practical solutions in experimental work - and for far-reaching solutions to problems of wide significance in his field. Another side of his personality is revealed by his interest in the early CBED efforts some twenty years before. He visited both G. Möllenstedt and Caroline MacGillavry when he was editing the book "Fifty years of Electron Diffraction" (IUCR 1981).

Peter Goodman and Gunter Lehmpfuhl met for the first time in October 1962 when he visited the department of Professor Molière at the Fritz-Haber-Institut in Berlin at the suggestion of Hein Wagenfeld. They were soon working together, and we would like to recount some circumstances leading to the success of that collaboration. Peter was working as a crystallographer in the field of electron diffraction. He was trying to record a larger area of the reciprocal space for a better comparison with theoretical considerations. He had the idea that this could be done by tilting the direction of the incident electron beam simultaneously with a shift of the diffracted beam on the photographic plate, as in x-ray diffraction. Such an instrument which could be used with slight modifications was developed in the department in Berlin. They followed the idea of John Cowley, who deflected the diffracted beam during photographic recording for a more accurate intensity measurement. The condition for a reliable analysis of the observation is that the recorded intensity distribution during the change of the direction of incidence is unambiguously correlated with a well-defined specimen area. It is very difficult to meet this condition. For such an experiment a single crystal specimen of uniformity in thickness and crystallinity with dimensions of several 10 μm was necessary. So they started with mica. The probability of investigating a uniform crystal area increases with the reduction of the beam diameter. Walter Dowell, who was working on his doctorate thesis in the department of Professor Ruska, drew the attention of Goodman and Lehmpfuhl to the fact, that a very small focus is produced in the back focal plane of the objective lens of an electron microscope, with a diameter of several 10 nm. So they tried to place the specimen in the electron microscope in this plane. But there was a problem: the back focal plane was not in the gap of the pole piece

but in the bore of the lower pole piece, 1.1 mm below the surface. Peter machined a cylindrical hollow screw, which could be inserted from above into the aperture holder of the objective lens. This was possible since they used the Siemens Elmiskop which could easily be separated above the objective lens. The lower end of the hollow screw carried a specimen grid with the crystal. Diffraction under such conditions is the Kossel-Möllenstedt technique. Very soon they understood why this diffraction technique was not generally applied. This was, namely, the contamination of the specimen when irradiated with such a small electron probe of high current density. Within a fraction of a second the brilliant diffraction pattern disappears and it is impossible to do a careful investigation. The contamination is produced by the interaction of the electron beam with hydrocarbon molecules on the crystal surface, replenished immediately by deposition from the residual gas of the conventional vacuum and by molecular migration on the surface. Gunter Heide, a member of the department of Professor Ruska, told them that specimen contamination could be reduced or avoided by heating the specimen. With this information, Peter mounted with araldite and conducting silver a small Pt-tape for heating in the specimen screw. The crystal was placed above a hole in this heating tape. The aperture holder and the adjustment screw were modified to feed in the heating current. Peter's art of skillful improvisation was fascinating, shocking their well-trained colleagues, but nevertheless solving a difficult problem. Later on the Pt-heating tape was replaced by a Mo-heating sheet, produced with a photochemical technique by Dr.G.Goldbach from the semiconductor laboratory of Telefunken. Now it was possible to investigate well-defined crystal areas by electron diffraction. The electron probe was formed by an electron beam with an aperture of approximately 1 degree. The aperture of this beam is determined by the diameter of the diaphragm in the specimen plane of the objective lens. With this geometry, the condition for the Kossel-Möllenstedt technique, automatically a large area of the reciprocal space is displayed, which would be tediously recorded by the combination of beam tilt for incidence and recording as described above. Small changes of the direction of the incident beam are possible by shifting the position of the aperture in the specimen plane of the objective lens. With this knowledge, Peter constructed, together with Jock Mills, a diffraction camera with an objective lens upside down, where the specimen, mounted on a goniometer stage below the lens, could be lifted into the back focal plane. Later he worked with an Elmiskop, modified for convergent beam electron diffraction and contamination control by Walter Dowell and Darryl Williams, in which the specimen and the surrounding area were cooled to 100 degrees K. Nowadays, such experiments can be performed in any commercial electron microscope with a condenser-objective lens due to Riecke-Ruska (twin- or

supertwin- lens). Specimen contamination, however, is still a problem which has to be overcome by appropriate treatments. These were the conditions for a systematic investigation of electron diffraction phenomena and for the quantitative analysis of intensity distributions for a comparison with theoretical considerations using the Cowley-Moodie phase grating approximation or the Bethe treatment for electron diffraction. Initially only the kinematical- or the two-beam- approximations were used for the interpretation of diffraction phenomena. However, with the development of computer techniques higher-order approximations could be used in order to study the crystalline structure of the solid state. Peter used the Cowley-Moodie approximation for simulation of the experimental diffraction intensities. The problem in the Cowley-Moodie theory is to vary the direction of the incident electron beam, and Peter solved this in an ingenious way by shifting the following slice in an appropriate direction in the thin-phase-grating-multiple-slice calculation. Gunter remembers Alex Moodie's pleasure when Peter showed the comparison of the experiment with MgO with his calculations with appropriate thickness, crystal potential and absorption. This had consequences for further investigations. (The energy of the electrons could be determined independently.)

Peter's interpretation of the symmetries appearing in CBED patterns, which was published in Nature (1974), opened up a new determination method of crystal point groups. The method was described in a very beautiful paper of Buxton et al., the Bristol group. The first result to be published (1964) from the work with Gunter was in fact the observation (or confirmation) of the condition for dynamical extinction in kinematically forbidden reflections. As Jon Gjønnes remembers, Peter was briefly back in Oslo some time in 1963, when he explained his experiment, and that he wanted some results to publish before he was due to return to Melbourne. He mentioned some nice CdS-crystals, and Gjønnes had suggested that his experiment would allow this condition to be observed in the forbidden 001-reflection of the Wurtzite-type structure. Which was what he and Gunter did, and they submitted the paper before Peter left. This is now the fundamental method used for space group determination. This was, of course followed by the other work on CBED-profiles for precise determination of structure factors - and on the deviation from Friedels law for determination of the full symmetry (beyond the classical 'diffraction symmetry'). The relation between the extinction lines and glide planes and screw axes was finally clarified by Gjønnes and Moodie. The formation of the extinction lines for all the space groups was later tabulated by Tanaka et al. Peter described the space group symmetry theory of the CBED method in the recent revision of the International Tables for Crystallography, Volume B.

Collaboration with Peter had a strong influence on the scientific development of many active researchers in materials science, especially that of Gunter Lehmpfuhl. Peter's intention was to compare experimental observations with theoretical considerations. With the development of modern computers higher approximations in theoretical treatments could be used in simulations for comparison with experimental observations. The agreement between prediction and observation and the sensitivity to several parameters was fascinating. So Gunter started to use computer techniques for the interpretation of the intensity distributions in rotating crystal experiments. This was the period in which the dispersion surface could be first recorded. It was a large step from using a slide rule for the interpretation of diffraction observations following the two-beam approximation to a more sophisticated computer treatment of many-beam interactions. When Peter and Gunter met first in Berlin, Peter smiled at Gunter's slide rule. He already used mechanical computers. But when Gunter came to Melbourne in 1965, he was shown a slide rule! However, at that time the large computer was already installed in CSIRO and Peter showed Gunter the first results of his many-beam calculations which Gunter tried to reproduce in Berlin in 1966. Back in Berlin in 1966 a diffraction camera, similar to the one constructed by Peter Goodman and Jock Mills based on Peter and Gunter's experiences in Melbourne, was constructed in the Fritz-Haber-Institut with the help of Harry Pühl.

In the years following the Berlin period Gunter and Peter were in more or less close contact. Because of health problems this contact could not be intensified as desired. However, there was a very fruitful exchange with colleagues working for some time in the department of Professor Molière. Gunter was also fortunate to be able to stay on two occasions for half a year at CSIRO, 1965 invited by Peter and 1984 invited by Walter Dowell.

Another person whose early scientific career was strongly influenced by Peter was David Cockayne. David first came to know Peter when he was sent as a student to help him and Alex Moodie build the early convergent beam electron diffraction camera at CSIRO in Clayton, Melbourne. David was advised that Peter had a heart problem, and that David's task was to relieve him of some of the workload. Anyone who knew Peter would know what an impossible task that was. From morning to late in the night, Peter constructed the instrument, with Alex as overseer and David as the apprentice. It was an environment full of enthusiasm and expectation, where a young researcher could not fail to be swept up in the pleasure of science. Peter was no tinkering scientist - he showed immense flair in designing equipment and experiments, he tackled the difficult problems, and he showed a mastery of experimentation that overcame technical barriers which would have stopped

most others.

Throughout his life, Peter was an enthusiastic mentor of young researchers. He did not have the formal skills of the teacher - indeed many are the anecdotes of his lecturing style - but he taught by example, and he was infinitely patient and attentive. Many young researchers benefited from his teaching, and he would go to great lengths to try to explain even the most difficult concepts.

There are many stories that are recounted about Peter, and we cannot possibly relate many here. The following anecdote noted by Colin Humphreys reflects something of Peter's character. Some years ago Peter and Colin were at a Conference in Japan. At the end of the Conference they went to the JEOL Electron Microscope factory and on leaving the factory both had a JEOL car for the very long drive to the airport. On the way to the airport Peter several times asked to know the time because he was concerned that they might miss their flight. Colin asked Peter if he had forgotten his watch and Peter replied that he had never in his life ever owned a watch! He went on to say that many people regarded him as absent minded, but a large part of this was because he did not own a watch and hence he was frequently late for meetings, late for dinner, etc. The Japanese salesmen in the car overheard this conversation Colin was having with Peter and immediately instructed the driver to divert from going to the airport and to call at a shop which sold watches. Peter mildly protested, but to no avail, and Peter selected a rather handsome watch. Colin does not now remember whether Peter or JEOL paid! We know that Peter was very proud of his watch and whenever Colin saw him in the future he would be reminded of this occasion and display his watch to Colin. We're not sure however that it made him any less absent minded!

Peter was concerned with space group determination until the end of his life. That is, he wanted to discover a distinguishing method of the two sets of space groups (I222 and I212121) and (I23 and I213), which Michiyoshi Tanaka had given up long ago. He eagerly proposed to Michiyoshi a collaboration to find a way to distinguish them in 1997. Professor Tanaka applied to the Ministry of Education of Japan for the financial support of this international research project and this application was accepted as a one year project in 1998. In October 1998, a colleague was sent to discuss their preliminary results with him, but unfortunately Peter appeared less vigorous for advancing the discussion. Just before his passing away and the end of the project term, Michiyoshi's team at length succeeded in solving the problem: the two space groups can be distinguished by the coherent CBED method. It was to Michiyoshi's great regret that he could not let him know the result. In his words - "I did not think at all that he ascended to heaven so

suddenly". It was a very memorable circumstance for Michiyoshi Tanaka to learn the CBED method from Gunter Lehmpfuhl using just the apparatus which Peter and Gunter had constructed. Michiyoshi felt at that time that the method was the last dynamical diffraction problem to be left unsolved and this problem was to captivate him to for over 30 years. He could not envisage his research life without Peter's pioneering work.

Early in 1983 the late Arthur Wilson and Uri Shmueli were planning Volumes B and C of International Tables for Crystallography. Since the old Tables dealt with X-ray crystallography alone, and the attribute 'X-ray' was now omitted, electron and neutron diffraction came in. This is how Uri first contacted Peter, the Chairman of the IUCr Commission on Electron Diffraction in those years. Largely thanks to Peter's valuable advice, electron diffraction is represented in Volumes B and C of the International Tables. Peter contributed to Volume B a section related to his own expertise: convergent-beam electron diffraction, and also participated, with Alex Moodie and John Cowley, in contributing to Chapter B.5.2: "Dynamical Theory of Electron Diffraction". Uri greatly valued his constant interest in the presentation of his material to readers, as evidenced by extensive revisions during the preparation of both the first and second editions of Volume B. Less than a year before he passed away Peter decided to replace his Section by a completely updated version and they started a new round of correspondence. Peter's plans were truncated by his illness but he never lost hope to resume his work, even a short time before his untimely death. Uri and Peter met several times during the 1984 Hamburg and 1987 Perth IUCr Congresses and had much more than casual exchanges of greetings. Peter was very kind, had a quiet but good sense of humor that Uri liked and respected him very much for.

Family contacts were very important to many of Peter's collaborators. At first in Berlin and then 1965 in Melbourne, where the Goodmans showed the Lehmpfuhl family the beauty of Australia, and also later in 1984/85, the Lehmpfuhl and Goodman families enjoyed time together. The last time both families met was in 1996. Gunter remembers very clearly when they spent two days in Christopher Creek, Arizona, after John Cowley's 70th birthday celebration. Gunter and his family are grateful for these family meetings and they will keep Peter alive in their memories.

Peter contributed in several important papers to the subsequent development of CBED-technique. But he appeared less interested in exploiting his ideas in a systematic way by perfections and applications. He will be remembered as an experimental pioneer, with an analytical mind that was immediately apparent to those who met him. He was, of course, also a product of the uniquely generous scientific environment that had existed in the

Chemical Physics Laboratory of the CSIRO, Melbourne. He was appreciated very much as a scientist, and as a friend.

Peter was not constrained by convention in his attitudes and outlook, whether at the level of the formal niceties of polite society or the politics of institutional hierarchies. He expressed a subversive sense of humour toward the display of rank in such structures and its attendant pomposity, and in some narrow-minded and intolerant environments he did suffer the consequences. Perhaps something like "dogged persistence despite initial skepticism" would be an appropriate phrase to describe his attitudes. Once Peter got an idea into his head there was no stopping him. Most of the students Peter supervised, including those recent students, have got a lot to thank him for.

His contributions to the field of electron diffraction and structural studies are indelibly written into the history of the subject, and will be abiding. His early convergent-beam work showing that dynamically-calculated intensities are well-matched by experiment opened up both the field of quantitative electron diffraction and the exploration of symmetries - leads which have been followed by other groups, including the fine work of the Bristol and Arizona and Norwegian Schools. Peter was an enormously valued colleague, who had deep collaborations with many of the leading diffraction theorists of the day, including Alex Moodie, Gunther Lehmpfuhl and Jon Gjønnes. His publications were always meticulously accurate and worthy of careful study.

He was a great electron crystallographer in pioneering the CBED method and his name will be definitely transmitted through the ages. We concur with the words of Michiyoshi Tanaka - "I pray for the repose of his soul".

David J.H. Cockayne
Jon Gjønnes
Colin J. Humphreys
Gunter Lehmpfuhl
John Murphy
Uri Shmueli
John C.H. Spence
Michiyoshi Tanaka
Nicholas S. Witte