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The Evolution of Crystallography from the Paris 1954 to the Bordeaux 1990 Congress

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This year, as in 1954, the International Union of Crystallography has chosen France as host for its General Assembly. It is tempting to compare the two events. Modern crystallography started in 1912 with its discovery by M. von Laue: thus the 1954 Congress took place just half way between the very beginning of X-ray crystallography and now. So it is a good time to compare what has been realized in an equal period before and after 1954 and to appreciate the evolution of crystallography. On the other hand, the two Congresses have given to the crystallographic community similar 'excitations', a third of a century apart. A comparison of the responses may reveal changes of mind in society.

The President of the IUCr in 1954 was J. M. Bijvoet. The Presidents of the Congress were M. and L. de Broglie and Ch. Mauguin. The Secretary of State for Research who presided over the Opening Ceremony was H. Longchambon. He was a crystallographer; so today is Hubert Curien. Of course, in between there have been many Ministers of Research who were not crystallographers, or even scientists. But we are proud to see that men whose great talents have been recognized have chosen crystallography as their scientific discipline.

The organizing Committee was chaired by Jean Wyart; we regret that he could not be with us today, as we had expected. J. Wyart told me that the finances of the Congress had been so well managed that he had been able to give some money back to the Union. We know now the reason for this financial success: the treasurer was a young man named Hubert Curien.

In 1954, the number of participants was about 500; it is 1700 in 1990. Quite a few who are with us today also attended the previous meeting. These representatives of the older generation show that they maintain their interest in crystallographic advances. The great increase in the number of participants is, of course, not surprising. We observe, however, that the growth factor is certainly less than the increase in the number of researchers in crystallographic laboratories or the increase in the number of annually published papers. This reflects a change of attitude of crystallographers towards Union Congresses. At the beginning of the Union (1948), crystallographers were working in a rather closed circle. Now they are working in laboratories for chemistry, physics, biology *etc.* in collaboration with colleagues of more and more varied backgrounds. Therefore, genuine crystallographers prefer to present their original works in specialized meetings: results discussed before specialists have a better chance to spread among interested people. For instance, in the early fifties, meetings in the domain of solid-state physics were rare whereas now plenty of them are organized each year.

So it is natural and, in fact, advantageous for a sound development of our discipline that the audience of the present and future Congresses of pure crystallography be self-restricted. However, periodical Congresses of the Union are essential: they are necessary because they bring together representatives of almost every crystallographic laboratory in the world. The success of the Bordeaux meeting proves that it fulfils a general need, to maintain the cohesion of crystallography and to facilitate the cross-fertilization of the various branches: somebody working in a laboratory for the physics of metals may find the solution to his problem in a paper by a colleague working with biologists. We can be reassured that there is no sign of a decline in the Union, even if the Congresses do not become enormous.

An important point is the partition of the participants from the different countries and also of the submitted abstracts. In 1954 the percentages were the following: UK 34, France 29, USA 12, Germany 11, Netherlands 7, Sweden 5 plus 21 countries below 5%. The striking feature is the predominance of the British delegation; the figure for France is distorted by the

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advantage of the host country. In the years after the war, as before the war, the UK appeared as the 'land of crystallography'. This was due to the influence of Lawrence Bragg and his school. Remember that the Union was founded in London (1946); its first President was L. Bragg; the first General Secretary was E. C. Evans from Cambridge. The participation of Americans was diminished by the fact that at that time crossing the Atlantic was not so simple - and so cheap - as nowadays. For Germany, one must remember that the war has been over less than 10 years. The contributions of the Netherlands and Sweden were very valuable, in spite of their rather small crystallographic community.

In 1990, the situation is very different. Germany is first with 19%, USA, France and USSR are together with 15-17%, then the UK with 10%; Japan 8%, India 5·5% and 42 countries below 5%. There is no longer one predominant country. In total, 49 countries are represented instead of 27 in 1954. Crystallographic laboratories are scattered all over the world and, as is natural, there are more researchers in the bigger countries. The interesting feature which emerges from the statistics is a general tendency towards the development of scientific research throughout the world, at least for our discipline which is outside 'big science',

Let us now discuss a more important point: the analysis of the content of both Congresses through the books of abstracts.

It appears that the centre of interest of the 1954 Congress was, on one hand, discussion of methods for solving crystalline structures and, on the other, their *description.* Patterson methods had been fully developed for a number of years. Direct methods had been initiated quite recently. J. Karle and H. Hauptman gave two theoretical papers and there were already one or two examples of the applications of direct methods. M. Perutz and L. Bragg presented a first sketch of the structure of haemoglobin but they were still far from a detailed structure of the biggest molecule which had been studied by X-rays. Neutron diffraction was just beginning. In the papers concerning electron diffraction, relatively more than nowadays, the possibilities of this technique were explored. The source of X-rays was the 'tube' similar to the present ones and, as detectors, photon counters were already used although the standard technique was still photography.

From the abstracts of the 1954 Congress, one gets the feeling that in the early 'fifties crystallographers already had at their disposal the apparatus and the fundamental theoretical methods that were needed to solve crystal structures. But the results were still at a latent stage, like the image on a photographic plate before development. What was lacking in 1954 was the computer. A few trials with the rare existing machines and some results were reported and one imagines that they were very astonishing at that time. Analogue machines had been built (R. Pepinski, G. von Eller); they were very ingenious but they became rapidly obsolete with the progress of solid-state electronics. Remember that the first transistor was built in 1948, only 6 years before the Paris Congress. The realization of the immense possibilities of crystallography occurred only after 1954 when laboratories had easy access to computers which were increasingly more powerful and well adapted to the needs of crystallographers.

There was a burst of important new results. One fact is very significant. Two Nobel Laureates, the founders of modern crystallography, M. von Laue and L. Bragg, attended the Paris meeting. In addition, in the audience, there were six future Nobel Laureates.* Of course, we hope that future prize winners are with us today, but we cannot ignore the reality that such an award is uncertain, at least for a purely crystallographic discovery. The time of the blossoming of the beautiful tree of crystallography may be over now.

The spirit of research in crystallography as well as the methods of work have profoundly changed. At the beginning, solving a structure was always long and sometimes very difficult. Often the main interest was overcoming these difficulties. Once a journalist asked Edmund Hillary, the conqueror of Mount Everest, why he climbed the Himalayan peak. Hillary replied 'because it was there'. Similarly, old crystallographers have often determined the structure of a crystal, 'because it was there', because they had at their disposal a good sample and a nice problem to solve.

Now the collection of the data and the calculations leading to the structure are more and more automated and they often become routine work which is no longer reserved for skillful specialists. The modern crystallographer must have a strong motivation to study a given crystal: its structure may be needed for the progress of the work of colleagues in other disciplines such as chemistry, biology, physics of solids *etc.*

Besides the computer, other new technical tools have considerably enlarged the possibilities of modern crystallography: new sources of neutrons, synchrotron-radiation sources, with surprisingly high power, linear or two-dimensional position-sensitive detectors *etc.* But techniques of the old type are not forgotten, because their simplicity gives them more flexibility. For instance, for the exploration of the reciprocal space of a crystal with defects in periodicity, the photographic method may be more efficient that the use of an automatic diffractometer.

It is important to emphasize that crystal structure determination corresponds to only one part of

* D. Hodgkin, H. Hauptman, J. Karle, A. Klug, N. W. Lipscomb, M. Perutz.

modern crystallography. There is also what we could call generalized crystallography, *i.e.* the study of the atomic structure of ill- or non-crystallized materials. At the Paris meeting, many papers were related to that subject. Today it is so important that it is the theme of one of the satellite meetings of Bordeaux.

This branch of crystallography has an essential character: direct methods are not valid when the positions of the atoms are not perfectly periodic. In other words, the problem of the phases of diffracted waves is not solved, and perhaps is not soluble. We are not able to deduce from the diffraction data through computer programs an image of a more or less disordered structure. So, as for crystal structures fifty years ago, the crystallographer must rely on his imagination or intuition to 'guess' models and fit them progressively to the diffraction data.

The evolution of crystallography has lead it to two neighbouring but distinct domains: studies of the ideally regular crystal on one hand and of ill-ordered condensed matter on the other, the degree of order varying from the good crystal with rare defects to the amorphous or glassy state. Thanks to the combination of theoretical and experimental progress, the precise description of the structure of the perfect crystal is a problem that has been solved. The remaining open questions are the understanding of their physical properties and, of course, their utilization. It is noteworthy that, at the 1990 meeting, one of the more important topics is entitled 'Relations of properties and structures'. Such a topic did not exist in 1954.

The study of ill-ordered matter has acquired a very important place in generalized crystallography, especially when there is partial order, as in liquid crystals, polymers, quasi-crystals *etc.* The advances are continuous, sometimes rather slow, because the problems are very difficult. Many substances with interesting properties have this type of structure and any new results are eagerly awaited by the physicists and technologists who study or use properties linked to the state of order.

Leaving now the technical aspects of the Congresses, we would like to point out some differences of a more general nature and, in the first place, its location in France. In 1954, when France had been chosen by the Union, Paris was the only possible place suitable for a large Congress. Apart from the Paris University there were no other venues able to accommodate a large conference with a department of crystallography large enough to form the nucleus of an efficient local committee.

In 1990 the situation in France has profoundly changed. One is able to appreciate the quality of the welcome from Bordeaux University, as well as the efficiency of the team of Bordelese crystallographers. Now, in France, several places have the possibility to host a large international conference. Paris is no longer the best place for meetings; it is always too crowded and expensive. In addition, it is often said that people in Paris have so many things to do that they have no time left to attend the sessions. The fact that the Congress is in Bordeaux today shows that the overcentralization of scientific activity in France has now been corrected. You are the witnesses of an important mutation which began in the early 'sixties.

Another remark, far less serious, is worth mentioning. The official dinner of the 1954 Congress took place in the magnificent Château de Versailles; the dinner was served in the beautiful gallery called 'l'Orangerie', but there was a strict condition: the guests were requested to wear evening dress (dinner jacket and long gowns). At that time such formality was accepted. I am sure that the reception offered this year by the Congress will be very pleasant. Certainly the organisers have many worries, but not, I presume, about the clothes of their guests. It is a detail, but isn't it a sign? 30 years ago, scientists formed a small limited group, with a little aristocratic touch. Nowadays, as anybody else, they feel free to prefer jeans to tuxedos.

In conclusion, I would like to quote an excerpt from the discourse of Ch. Mauguin at the opening ceremony of the Paris Congress: 'Une connaissance complète des phases permettrait une solution automatique qui pourrait être effectuée par un robot. Les résultats, certes, garderaient tout leur intérêt, mais on n'aurait plus la joie de la difficulté vaincue pour les trouver'. (The knowledge of phases of diffracted beams would allow automatic solutions which could be carried out by robots. The results, of course, will keep their interest, but one would no longer have the joy of mastering the difficulty of getting them.)

Well before the computer era, Ch. Mauguin made a correct prediction about the coming revolution of the work of crystallographers. In his time the quasi-automatic solutions of crystal structures were a mere dream. But he was pessimistic about the negative effects of computers. We know now that the problems facing crystallographers have only changed not disappeared. Some have vanished but new ones have appeared which require reflection and imagination and which in turn may still, for a long time, bring much joy to all those who like crystallography.