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Powder and single crystal x-ray and neutron scattering / Magnetism / Oxides presenting remarkable properties: superconductivity, giant magnetoresistance, charge, spin & orbital ordering / Computer programming and data analysis / Neutron diffraction instrumentation

1. What is crystallography

Crystallography is an inter/trans-disciplinary field of science that embraces many (every?) things concerned with the study of the *structure* of matter at atomic and mesoscopic/macrosopic level. This last part makes reference to crystal growth, morphology and co-operative self-organisation of matter. Crystallography uses and develops some aspects of mathematics concerned with the symmetry of spatial arrangements of atoms and magnetic moments (electron and spin densities). Mathematics is present in all crystallography aspects concerned with *methods* and *procedures* to exploit experimental data in order to get structural information. Crystallography relies mostly, but not exclusively, on diffraction physics that is at the basis of experimental techniques providing information about the structure of compounds. The results of many crystallographic studies (structure determination) have an enormous impact in chemistry, metallurgy, geology, mineralogy and biochemistry. The major part of crystallographers is probably working on some of those fields for solving crystal structures. It is probably this last aspect that gives to crystallography, when seeing from outside, the *instrumental* character it owns.

2. Is there a better name that could replace the historical term “crystallography”?

The only name susceptible of competing with the traditional term is *structural science*, however this seems to be a much broader concept. Is the study of gases, liquids and amorphous materials within crystallography? Most concerned scientists will answer *no* to this question. I consider, however, that the methods, experimental techniques and problems of disordered matter are similar to those found in the study of defective crystals or non-periodic arrangements of atoms (quasicrystals). The structure and properties of disordered matter should be part of the common knowledge of crystallographers. For me, the name of *crystallography* is an adequate term to describe the aspect of structural science dedicated to quasi-ordered forms of matter.

3. What are the most important unsolved problems in crystallography?

There are unsolved problems in crystallography, but there are more in physics/chemistry (metal-insulator transitions for instance) or biochemistry (protein-protein recognition for instance) that crystallography may help to solve.

For me there are several specific problems in crystallography of practical importance (even if they are presently tackled with available methods), for instance:

- Automatic indexing of multiphase powder patterns.
- The automatic solution of macromolecular structures.
- Convenient ways to describe non-periodic structures and the calculation in a closed (finite) form of their diffraction pattern. The superspace approach is an elegant answer for quasi-periodic cases.

And other more conceptual

- Prediction of the structure of new materials: what is (are) the structure(s) of a compound given its chemical formula? In case of polymorphism, what is the sequence of stable structures?
- Is there a maximum number different chemical species in ordered structures?
- Mechanisms and driving forces of first order phase transitions.

4. What is the future of crystallography? Is there any future?

I think crystallography has a bright future in spite of the current situation, concerning teaching, in many European countries. At present, it is bio-crystallography the most in fashion sub-field of crystallography. This is so because of the present huge impact of biological and medical research in the advanced countries. Politicians and decision makers are driving and favouring a research that is important in the understanding of key aspects of the chemistry of life and the consequent production of pharmaceuticals against lethal diseases (cancer, AIDS, etc).

On the other hand, the availability of high performance synchrotrons and high flux/resolution neutron diffractometers are changing the character of the results. For instance, a) the study of electron and spin densities are now much more precise, b) the study of structures in extreme conditions (temperature, pressure, electromagnetic fields) becomes now possible, and c) *in situ* diffraction of transient states (chemical reactions for instance) is now reaching a quasi-routine status. New fields are being opened thanks to the availability of these techniques.

The treatment of the enormous amount of data produced in 2D + 1D detectors (surface detection plus time) of new diffractometers demands even faster computers and graphic user interfaces to handle efficiently the information. Together with the data-treatment aspect, computer modelling and simulations are needed. Computing programs are obviously needed for solving and refining structures, however, with the increase of complexity, simulation techniques and modelling are becoming of utmost importance in crystallographic work.

Crystallography will continue to play an important and increasing role in the study of the relation structure/properties in condensed matter.

5. Should we still teach crystallography? Why and how should we teach?

Of course! Crystallography should be taught within the traditional faculties. I think the study of crystallography should be reinforced. It is clear that material science and biology will need more and more precise crystallographic studies because the knowledge of the structure is the first step in understanding the behaviour of materials and biological molecules. The ever-increasing complexity of new materials and molecules demands well-trained crystallographers to tackle new challenging problems. Departments of crystallography should be encouraged where physics, chemistry, geology and biology faculties are sharing a campus. This kind of interdisciplinary grouping may be of great importance to make efficient and productive the intercommunication between specialists in different fields.

6. Personal recommendation to a student who wants to enter into crystallographic research

I would recommend to him (her) to increase his (her) training in:

- a) Fundamentals of crystallography: symmetry, space groups, structural types, diffraction, phase problem, direct methods, . . .
- b) Applied mathematics: symmetry analysis, algebra, Fourier techniques (FFT, wavelets, . . .), simulation techniques, programming . . .
- c) Diffraction physics: scattering theory, x-rays, neutron and electron diffraction. Diffraction by real crystals, defects, different experimental techniques.
- d) Chemistry. Depending on the particular field:
 - Material science and solid state physics and chemistry
 - Organic Chemistry and biochemistry
 - Mineralogy

To be prepared for hard work, to go beyond the routine tasks, not trust on black-boxes software; learn programming, algorithms to learn still more. All these things are extremely useful for whatever field in crystallography.

7. What is the impact of crystallographic research? What would you tell your funding agency or the president of your university? What would you tell the taxpayer?

I have already stressed the important impact of crystallography in nearly all fields of science concerned with the structure of matter. To the funding agency I will tell to be careful with the excess of favouring only “in fashion” or supposedly applied research fields (the use of “nano” and/or “bio” prefixes seems to be necessary for getting financial support everywhere). Support to fundamental research is of paramount importance if we want to go beyond what is already known. That is what I would tell to the taxpayer.