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Automated Diffractometry

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A review of the status of automated crystallographic measurement has shown that, other than in the mechanics of data measurement for structure determination, little research use is being made of the power of algorithmic, programmed control of diffractometers. Rather, existing computer-based systems are being used largely as non-interactive sequencers. This appears to be due to a lack of a strongly perceived need coupled with frustrations over the awkwardness of the man–machine interface, weaknesses in the programming languages, and doubts concerning the basic utility of automated diffractometry. However, possibly valid applications are outlined for such studies in crystal physics as those dealing with radiation damage, handling measurements near phase transitions, studying extinction in small crystals, sensing the unexpected, and detecting and eliminating artifacts. The lowered cost of computing equipment and more widespread use of higher-level languages are suggested as improving the future prospects for automated diffractometry.

Introduction

The NAS-NRC Committee on Chemical Crystallography recently asked me to take a retrospective look at the status of 'automated' diffractometry. (The term 'automated' is used here to connote the full, on-line control of the experimental process by a computer. It implies not only the programming of the sequential measurement steps but, more importantly, the 'programming' of the actual course of the experiment itself, in which decisions are taken and process branches made in response to the real-time analysis of the data.)

The request came to me because some eleven years ago I led a group which designed a large, computer-controlled, multi-diffractometer operating system (Beaucage, Kelley, Ophir, Rankowitz, Spinrad & Van Norton, 1966). The system was emplaced to handle the experimental needs of a group of eight neutron diffractometers at Brookhaven's High-Flux Beam Reactor. In addition, it controlled the operation of an X-ray diffractometer located at the same facility.

The system was designed to allow complete programmatic control of the experimental process. The research worker could not only direct the apparatus through the classical measurement sequences but could also interpose data reduction and analysis steps to alter or redirect the course of the experiment, in real-time, in response to the data thus far collected. The underlying notion was that the crystallographic arts would be advanced if the experimenter had this kind of automated mastery of both the mechanical and computational (or algorithmic) aspects of the measurement process.

The system was, at the time, considered to have great portent for the future of crystallographic research.

Ten years later

Last year the Brookhaven High-Flux Beam Reactor celebrated its tenth anniversary. It seemed, therefore, a reasonable time to revisit our expectations for that system – and for the many like it that have been put into operation in the last decade. [Sparks (1973) has presented a brief overview of some of these systems.]

Has automated diffractometry met its promise? Has the on-line computer significantly altered the way the research scientist works? Yes and no. 'Yes' because for the chemist or physicist interested in reasonably straightforward structure determination, the automated diffractometer has been a labor-saving boon. [A review of computer-controlled measurement procedures is given by Sparks (1976).] 'No' because in my discussions with workers in the field I have learned that, although many use computer-controlled diffractometers, few exploit their capabilities for algorithmic, decision-making management of the experimental process in their more physically oriented crystallographic studies. Most interestingly, this pattern of use does not derive from an inability to manage the details of computer guidance but, rather, from a lack of interest in it. The capabilities that seemed important, in prospect, ten years ago have, in retrospect, faded from significance.

Why is this? Why did the desire (not the promise) fade? Some answers can be given.

Impediments to effective automated diffractometry

As indicated above, the dominant reason for the low utilization of programmed control is the lack of compelling, experimental demand. If programmed control were really important to the experiment, the scientist would employ it. (The capabilities are acknowledged to be there.) So the reasons for lack of use outlined here must be viewed more as impediments than as absolute barriers. Two problems were repeatedly referred to: the awkwardness of the man-machine interface and the absence of a convenient programming language.

The time-consuming difficulty in getting things done; the inability to smoothly alter or add to a programmed procedure; the arcane computerese – all of these were cited as tending to discourage the experimenter from using the system's capabilities. In many instances it just seemed easier to do things either manually or within the constraints of the existing procedures than to spend so much time in order to 'save time'.

The second frustration referred to was the irritation and difficulty in learning and working with the rather rudimentary programming languages which most of the systems demanded. This frustration had two aspects. First, there was the basic annoyance at having to learn an otherwise useless language discipline. And second, the language, once learned, was so primitive with respect to the crystallographer's needs that 'programming' the experiment became a very tedious procedure.

Inappropriateness of automated diffractometry

A second theme ran through the remarks of the crystallographers to whom I talked. It related to the possible fundamental inappropriateness of automated diffractometry. The argument ran this way. The scientist should commit his or her experiment to the 'hands' of an automated system only when he or she is sure that there are no surprises left. That is, such a system should be invoked only after the crystal has been broadly explored and is ready for more detailed measurement.

That being the case, the argument goes, the only appropriate programming – beyond that of the straightforward measurement sequence – would be that directed at detecting anomalous events or data trends. But the detection of such circumstances invariably signals the need for manual intervention anyway. So the 'automatic' experiment would be unable to proceed until the scientist stepped in and corrected the problem. (Recementing a loose crystal, for example.) So why bother?

Possible applications

While these points of view are understandable, the situation is not that clear-cut. There are, in fact, justifiable ways in which automated diffractometry can be used (Abrahams, 1975).

Dealing with radiation damage

The onset of radiation damage can be sensed and the data collection strategy altered. (The physical environment of the crystal can be changed, for example by lowering the temperature. This could be done under computer control by cooling the crystal to a temperature at which the experimentally-detected rate of radiation damage becomes just acceptable.)

Handling measurements near phase transitions

Electric field, magnetic field, temperature, pressure can be programmed singly or in combinations to suit the experimenter's purposes.

Experimental studies of extinction in small crystals

Wavelength dependency can be studied through computer manipulation of the radiation sources. (See a group of three review papers on extinction presented at a Commission on Crystallographic Apparatus Open Commission Meeting in Amsterdam in August 1975: Becker, 1977; Lawrence, 1977; Schneider, 1977.)

Sensing the unexpected

Scanning for unexpected scattering phenomena – important to assure the quality of the results – can be readily, and intelligently handled by programmatic control. (Unexpected weak but sharp maxima at points in reciprocal space, either commensurate or incommensurate with the principal lattice, or continuous regions of diffuse scattering, should be detected and either flagged for attention or measured.)

Detecting and eliminating artifacts

Diffraction profiles of formally equivalent reflections

even for spherical crystals often exhibit differences of shape or integrated area beyond that expected statistically. Contributing errors as a result of multiple scattering, improper sampling of diffuse scattering *etc.* can be investigated programmatically by rotation about the scattering vector or change in the scan mode.

Future trends

Certainly more can be done than is being done. Hopefully, more will be done. Certain trends argue for this.

First, the radical and continued drop in the cost of computing equipment will put this kind of apparatus into the hands of a larger number of experimenters. Those who already have automated diffractometers will find that costs are dropping so rapidly that they will be able to afford substantially larger on-line memories. That, in turn, translates into substantially more sophisticated and versatile control programs.

A second trend is towards the kinds of control and programming languages with which crystallographers are comfortable. The system of which I spoke at the beginning of this paper is now in the process of being extensively upgraded (Dimmler, Greenlaw, Kelley, Potter, Rankowitz & Stubblefield, 1975).

One of the prime motivations was to provide Fortran as the programming language. Others have followed the same route (see Sparks, 1973, 1976).

However, what is needed is a coming together of crystallographers to agree on common conventions and standards for their systems. In this way future systems can be built to stand on the shoulders of their predecessors and not their toes.

In 1967 I wrote a paper (Spinrad, 1967) in which I tried to explain how the research laboratory was becoming automated. I reviewed the underlying principles, offered examples of current systems and extrapolated future trends. One of the examples I used was that of automated diffractometry. Regretfully, of all the fields reviewed, crystallography has made the slowest progress. Other fields have substantially realized the potential that was apparent in the 60's. But, except for some advances in the mechanics of structure determination, crystallography has not. I hope that this will change. There is really no reason why it should not.

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Criteria for Selecting and Interconnecting Micro, Mini, Midi and Maxi Computers

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Four commonly accepted computer classes today are: micro, mini, midi and maxi. The dominant parameter which gives rise to this categorization is price, which varies from a ten dollar microprocessor chip to a ten million dollar maxi. This paper attempts to identify other parameters associated with each class in order to provide a mechanism for determining optimization of computer use. Trends towards increased parallelism at both ends of the spectrum are discussed. Finally, a method is described for interconnecting all classes of computers and peripherals at a site to form an installation network.

Introduction

The author's background includes the design and systems application of maxi computers over many years and recently the design and application of microprocessors. This experience led the author to concentrate the main thrust of the paper on the two ends of the computer class spectrum.

The computer structure classification of micro through maxi is one adopted by the trade journals