has been 'swamped' by a very strong reflexion. The 5-point check system referred to by W. Hoppe has proved most valuable in detecting drifts, *e.g.* in goniometer heads due to thermal gradients. Since the operational region has been thermostatted these effects have been greatly reduced.

FURNAS: Particularly with instruments which have a long path length it is necessary to consider not only changes of temperature, but also of barometric pressure which occur during the experiment and alter the air absorption.

LADDELL: With a crystal monochromator, the high intensities referred to by Rogers do not occur and hence the probability of photomultiplier 'fatigue' occurring is correspondingly less.

JENNINGS: Our experience with photomultiplier tubes may shed some light on the point raised by Professor Rogers in connexion with changes in detector sensitivity after exposure to high count rates. We have found that such exposure can change the gain of the photomultiplier for many minutes. Such gain change can cause an appreciable fraction of the pulses to lie outside of the acceptance of the pulse height analyzer. There are similar changes in gain across the face of the photocathode and it is necessary to take cognizance of these for the most accurate work. It is our experience that the more recently designed photomultipliers minimize these effects, but do not completely eliminate them.

ROGERS: There are important restrictions in mounting triclinic crystals if there is only a quarter circle. On the other hand, the obscuration produced by the goniometer head can be quite large and may nullify the advantages of a full circle.

WOOSTER: It may be an advantage to construct the χ-circle as a full circle, even though one only uses part of it. We have constructed a small goniometer head which produces minimal obscuration.

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Error Evaluation *versus* 'On Line' Correction

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Crystallographers have enjoyed a freedom of access to computers that cannot continue. In spite of widespread pressures to automate experiments, computers are not a substitute for proper experimental technique. As a group, crystallographers are remarkably naive not only regarding the evaluation or comparison of the experimental and computational techniques which they employ, but also regarding the actual cost and value of their efforts. Some concerted thought, effort and self-education must be undertaken soon lest extravagance endanger future support.

Introduction

The art of crystal structure determination has and seems always to be of interest to at least two widely divergent groups of people. The first and far more numerous is composed of those whose interests are primarily chemical in nature, who for many years have been delighted with the ability to write structural formulae on a flat paper and for whom three-dimensional structural information is and will be a great and appreciated improvement often containing far more information than can be used, explained, or even comprehended by their majority. The second group is composed of those whose interests concern details such as bonding electrons, anisotropic or anharmonic motions of atoms, interatomic distances and angles with high precision and accuracy towards a better understanding of molecular structure and the solid state. Yet, there are a growing number of persons whose interests oscillate between these extremes and it is good that through them, we may be better able to assess the needs of each and the role to be played by this assembly of 'experts in the field' toward realistic solutions.

The convenience of large computers and the ingenuity of mathematicians and programmers have in many instances far overworked the experimental data available in an ever tightening spiral toward a 'better R factor'. There has been dangerously little attention given to the actual cost of the overall operation and the value of the result obtained beyond the intellectual and status satisfaction of 'having gotten an R factor below 5 or 3%', *etc.*

It is unfortunate, but true, as many of our colleagues are telling us at this very meeting, that our understanding of many of the experimental parameters that enter into and affect the data are so far out of our grasp that we are genuinely unprepared to do an honest job of 'on-line correction'. We are unable to describe in concise, reproducible, and understandable terms all the criteria for performing a valid experiment whose resulting data will have the meaning intended and be the object of worthwhile expenditure of effort to any specified precision or accuracy. By this it is implied, as stated before, that much expenditure of time, effort and money in the past has *not* been worthwhile. It is also implied that we are essentially unable to point a finger and say what parts of those expenditures were *not* worthwhile. It is further implied that this assembled group must come to grips with and delineate rather clearly the facets of the problems involved toward their solution. To do otherwise constitutes a mockery of our profession and of our financial supporters.

I am reminded of the comment made in 1965 at the ACA meeting at Suffern, New York, by Dr. J. Ladell to the effect that we must not let the idea of 'on-line correction' become a substitute for proper experimental technique.

In accepting the invitation to speak to this assembly, I wrote thus to Dr Sidney Abrahams:

'I very strongly believe that we know too little about the vast array of known and possible sources of errors to allow crystallographic structure determination to be left to the whims and fancies of programmers, to the availability of time or programs bearing seemingly appropriate labels or brief descriptions, to the slovenly practices of those who believe (quite falsely) that anything can be corrected by using a computer, to those who act as though numbers can be pushed around *ad-infinitum* but who aren't to be bothered about where the numbers came from or exactly how they were obtained.

'We must arm ourselves (1) with an understanding of the parameters that interact in the experiments wherein data for crystallographic structure determinations are obtained, (2) with expressions for the effects of their independent variation, (3) with expressions for their interactions in simultaneous variation, (4) with expressions or evaluations of the limits that can be tolerated in any one or any simultaneous set of variations with respect to their effects upon results or various kinds of interpretations to which the results may be subjected, (5) with some independent means for evaluating a set of raw data, a set of partially corrected data or a set of 'fully corrected' data (whatever that might be!), (6) with some genuine criteria by which a valid experimental procedure, arrangement and alignment can be defined, specified and achieved, (7) with some genuine criteria by which an *invalid* experimental arrangement, alignment or procedure can be detected, determined, defined and corrected, (8) with the guts to face the consequences of the fact that correction, it seems to me, generally will require 'on-site' mechanical, electronic or related operations *before* the final data to be used are collected and *not* by the performance of special procedures or manipulations of 'so-called' data after it has been collected.

'We must be prepared to severely censure those who violate rules of correct experimental procedures. We must also, to attain definitions of what those are, encourage critical work toward the evaluation and comparison of experimental procedures, but here again they must be balanced accounts of known as well as any newly discovered variables and their effects. For example, works describing the stability of an X-ray generator in terms of measurements of the emitted beam intensity without regard for the effects of changes in air density in the given path length or for the effects of changes in ambient temperature upon the detector or associated electronics, or for the effects of stability of the pulse height analyzer, *etc.* or *etc.*, *must* be suspect.

'I sincerely hope that the several speakers on detailed sources or areas of error will take to heart this assignment to prepare ourselves for the onslaught of computer controlled 'data-factories' and to underline the need for a proper fundamental training of operators (and owners). Otherwise we face the bleak future of an explosion of 'structures' and of 'disputes' whose existence will not only clutter the vastly increasing volume of literature with error upon error but also waste both the original investigator's time and the time of those who follow in repeated redeterminations in efforts to clarify the irretrievable.'

Thus was set the tone of my considerations in approaching this meeting and in listening to the papers thus far presented.

Yesterday, Sir Lawrence Bragg (Bragg, 1969) described to us the status of X-ray intensity measurement capability in 1914. In many respects it rivaled what most of us are doing today. Why should this be?

I cannot really answer this question other than to observe that for one mad reason or another we all have been swept along in time too preoccupied with being occupied to pay enough attention to what was and is really happening.

For example: During the teens, much work of great use and significance was done in X-ray spectroscopy and in X-ray intensity measurements as well as in the elucidation of theoretical bases for the observations already made or predicted (Ewald, 1962; Bragg, 1969).

Attention soon turned to more complicated structures, the diversion to photographic techniques because of the tedium inherent in ionization chamber measurements, the relaxation and essential 'basking in the sunshine' of many more data points than parameters, thus (except for the tedium of visual estimates of intensities and the use of Beevers & Lipson strips) the ease of structure determinations satisfactory for the purposes then to be fulfilled.

Upon the development of new technologies – the Geiger and proportional counters, the diffractometer and the era of commercial devices – the interest and frenzy for 'more of the same' produced two-week concentrated courses in X-ray diffraction, many practitioners and few experts.

Then the real blow fell – before any real progress was made to reduce the tedium of data collection (and therefore before any programs for study or evaluation of experimental techniques could be undertaken reasonably), computers suddenly allowed an almost infinite variety of manipulations to be performed on the many reflections (even though known only as weak, medium, or strong) which considerably overdetermined the structural parameters.

Recently the table has turned and the capability of collecting large numbers of data in reasonable periods of time is becoming widespread. Now, combined with the existing computing capabilities, it is certainly time for us to take time to examine what we are really doing with all this expensive and powerful equipment.

In all honesty, it is largely a 'more of the same' situation in which numbers, however obtained, are cycled repeatedly through very sophisticated computers, too often in quest for a 'better R factor' without regard for the fact that said computer time actually costs someone a lot of money, for the fact that the original set of numbers may have had no greatly significant relation to any reality or for the value of said structure either to the inquiring scientific community or to the investigator's employer.

I may cite some examples: One academic laboratory did a structure determination for an industrial firm charging only for the actual time and salaries involved, no charge for having had the equipment or a place for it. The cost was $10,000 *before* refinement. The academic laboratory did refine the structure 'out of curiosity', but did not even attempt to charge for said refinement because the customer was so shaken by the $10,000 bill. (Incidentally, the structure contained approximately 50 atoms in the asymmetric unit, hence this represented a remarkably low cost of only $200 per atom.)

In another firm equipped to perform their own work, the annual operating costs (excluding amortization of the equipment) exceed $150,000 per year and by running their equipment over 6000 hours per year they are able to determine about twelve structures per year. On the whole, these were smaller molecules than the previous example so the average cost could be described as twelve thousand five hundred dollars per structure or about five hundred dollars per atom – plus having the capital investment.

In the United States, costs are actually somewhat higher than this, such that, in 1968, on the basis of a 2000 hour work year for the staff, data collection alone costs about $75 per hour, to which must be added the costs of computer time now generally in the neighbourhood of 20 cents per second or $700 per hour.

Certainly some structures are more complicated than others – last year at Atlanta, Georgia, we were told that ribonuclease cost over $2,000,000 and 16 years of effort by many people *just* for the crystal growing and X-ray work! How much more was expended in the chemical determination of the amino acid sequence is probably incalculable.

We have enjoyed unusual freedom both with respect to the use of computer time (we even have had inquiries from firms having computers and not much to do with them concerning X-ray diffraction equipment 'because they had heard it could use a lot of computer time') for which even universities now are having to take a closer look at the actual costs and the results obtainable during the available time – and teaching undergraduates 'computerology' is a growing consumer of university computer time – and with respect to the unique role occupied by X-ray (and neutron) diffraction techniques toward the elucidation of three-dimensional molecular structures.

In these times of scarce money we must be careful not to overstretch credulity in our demands either for equipment or for computer time. We must, on the one hand, relate our efforts to the genuine needs of the industries that support us, and on the other hand, take this unusual opportunity to regroup and perform the long overdue experiments that will permit the definition of experimental parameters that are necessary prerequisites to valid data and worthwhile analyses such that the occasionally longer range views of academic institutions and government support agencies can be fulfilled with the promise (and performance) not only of better quality, but also of some criteria of economic value.

We have already heard some of the problems mentioned both in experimental and in theoretical areas. We shall hear much more, but this is not sufficient. We must here resolve and indeed attempt to define some of the experiments that must be performed not only to advance our knowledge and understanding, but also to form the basis for further 'monoparameter' sets of experiments and their further basis for more theoretical work.

Perhaps I should cite some examples:

I. With respect to the X-ray source:

A. Its stability: is a constant voltage and current sufficient or must the output be monitored?

We have never been able unequivocally to relate output variation to any of the often cited 'wandering focal spot' or 'tap water temperature' stories.

B. Its intensity distribution: There is no substitute for a photograph to show what a focal spot looks like. But pinholes must be suspect; therefore, use the crossed cylinders described recently by Parrish (1967) and used for several years in our equipment. Note further that the apparent intensity distribution may be not only a function of take-off angle but also of the wavelength. Films are not discriminating and scans of the images with a detector are a little more tricky than implied by Parrish.

C. Its nature: Is it diffuse such as from a fluorescent or electron excited target or is it directed as from the virtual source when a crystal monochromator is used?

D. Its spectral output: There are both gross and detail differences which are functions of the target material, the take-off angle, the operating voltage (and whether that be A.C., full wave rectified, merely capacitor smoothed constant potential, or ripple free D.C.), the window material, *etc.* (Gilfrich & Birks, 1968).

Striking apparent differences arise from the detectors used to measure the spectral output. Here the necessity for some considerations in addition to the mere absorption characteristics of the detector come into play as shown by Fig. 1*A* and *B*. I do not know why a change in scintillation crystal thickness should produce at the 33 keV absorption edge the completely opposite effects illustrated. It was with these curves and others obtained under different tube operating conditions freshly in mind that I heard Professor Parratt of Cornell address the Pittsburgh Diffraction Conference in November 1961 regarding the effects of operating potential and voltage current wave shapes and phase relations upon spectral output and even details of spectral line shape. I am sure that these experiences have contributed markedly to my concern regarding generator stability, detector performance, other experimental parameters and the interpretation of data.

II. With respect to detectors we must further mention such things as:

A. Stability of their high voltage supply
B. Stability of pulse height distribution with count rate, *etc.*
C. Sensitivity, spectral as well as absolute (and efficiency)
D. Inherent counting rate limitations (more often in the associated electronics rather than in the detector itself)
E. Uniformity of response across its area and the methods for mapping

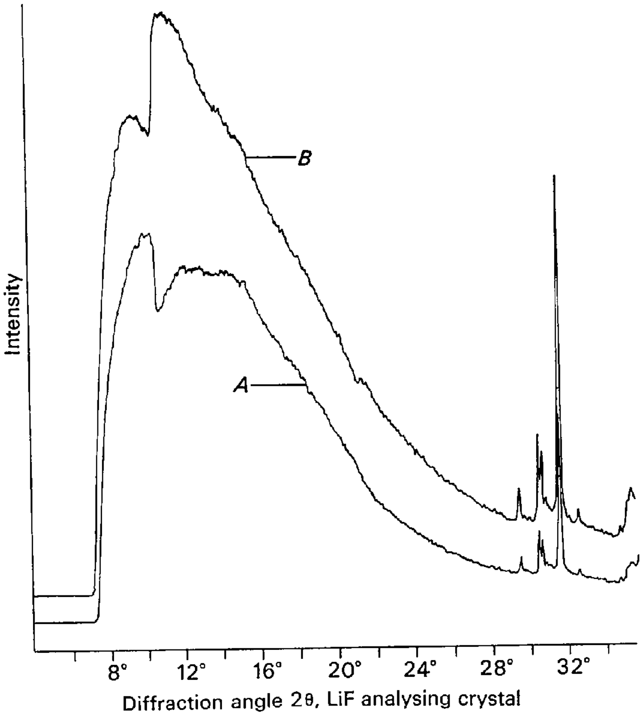

Fig. 1. Effect of NaI(Tl) crystal thickness on recorded X-ray tube apparent spectra. Curve *A*, 0·030″ thick; curve *B*, 0·500″ thick.

III. What does a reflection look like?

Fig. 2 (which is similar to Figures in the ACA Transactions, Volume I of the Suffern, New York meeting in February 1965) shows how this depends upon the manner of measurement. 2 *A* is a stationary-crystal photograph of a reflection as it appeared at a point in time. 2 *B* is a 2θ scan of the same reflection. Here the film moved with the detector so the record is in essence the source. 2 *C* is an ω scan of the same reflection. In this case the film was stationary such that as the crystal rotated the $K\alpha_1$ and $K\alpha_2$ reflections appear side by side. These three photographs illustrate the often committed fallacy of balancing left/right intensities to center a reflection (after having matched top/bottom): although that is how I described doing it in 1957.

You will note that I carefully excluded from that manual (Furnas, 1957) any real description of how to determine lattice parameters from a real specimen. I did not know then and I am not sure that I do yet.

Yesterday Dr. Diamond (Diamond, 1969) described the use of profile analysis. I believe that some preliminary data on the crystal, including its physical dimensions and shape relative to the reciprocal lattice direction could be valuable input to his routines since certain aspects of the variable shape of reflection can be predicted.

I have often thought an inverse process could be used to permit more accurate determination of lattice parameters from single crystals.

Returning to the L/R device – one never knows what part of the source is being used by the crystal. The source is as large as is shown in Fig. 2 *B* but which part is being used for the photograph in Fig. 2 *A*?

Further, if there is dispersion (or at moderate and high 2θ angles), one never knows what wavelength is responsible for the determined 2θ position.

There further exists no unique set of ω, 2θ, $(\chi+\varphi)$ coordinates for a L/R balanced reflection.

Better results are obtained after matching T/B, using a narrow source and by progressively symmetrically narrowing the receiving aperture, tuning both ω and 2θ while so doing. This not only generally forces one to the peak of the $K\alpha_1$ reflection, but the ω width and intensity variations observed during said ω tuning operation provide an answer to the important question of crystal mosaicity. Just as a streak on a Weissenberg film shows specimen mosaicity, the narrowness of the streak demonstrates the unique 2θ value associated with the *d* spacing which may be (and often is) quite independent of mosaicity.

Actually, the specimen is always a monochromator; so that the way it views the source, whether real or virtual, and what it outputs to the detector is only a first description of a monochromator.

If a monochromator is used either in the input or emergent beam, then the experiment must be considered as a ‘mismatched’ double crystal spectrometer. There

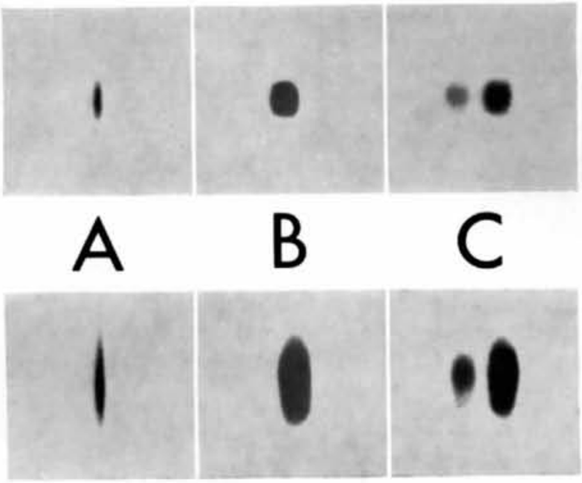

Fig. 2. Comparing the 531 reflection of Cu $K\alpha$ from CaF_2 using direct beam (top row) and a mosaic graphite monochromator in (1, *P*) orientation (bottom row). Column *A*, stationary crystal stationary film; *B*, 2θ scan; and *C*, ω scan.

are significant differences between parallel and antiparallel arrangements where the dispersions respectively subtract or add, hence are not symmetrical about the incident beam direction, or in the perpendicular arrangement in which the dispersions are independent (since perpendicular), hence produce diagonal spectra symmetrical about the incident beam direction. This perpendicular arrangement has several advantages described first at the Gatlinburg ACA meeting in June 1965 (Furnas & Beard, 1965) but otherwise essentially unpublished.

The result obtained when one or the other crystal in any of these configurations is 'moved' is different as to whether it is the first crystal or the second crystal that is moved – as is usually the case with a mismatched double crystal spectrometer. The perpendicular arrangement avoids many but not all the problems that may arise.

At this point one might note that in the use of a crystal monochromator to assess the polarization of the X-rays diffracted from a specimen, it is necessary to use and combine data from what are effectively all the arrangements described above. The mere observation of intensity differences and their agreement with some expected result are not *a priori* proof that the quantities measured actually had just the meaning ascribed to them. It is strongly urged therefore, if polarization assessment techniques be used that they not be spoiled by the crystallographer's traditional reliance upon single measurements.

The real problems with respect to using monochromators are little appreciated, poorly understood and are substituted for the more commonly recognized problems with non-monochromatized radiation. We do not presently know their full import, magnitude or effects. One can only advise caution tempered by the observation that to the usual precision to which data is collected and understood today the reduction in background and improvement in signal/noise ratio seem well worth the risks.

Fig. 3 shows the perpendicular arrangement of the monochromator together with a goniostat for single-crystal data collection. It is with such a combination that most of our data are now being collected (Furnas, 1965).

Fig. 4 shows an experimental arrangement which Mr D. W. Beard and I described at the ACA in Minneapolis in 1967 (Furnas & Beard, 1967; Beard, 1968) in which the monochromator mechanism was mounted on to a diffractometer supported against a vertical column such that the axis of the diffractometer coincided with the emergent beam from the monochromator. This beam then impinged upon a specimen in a usual goniostat with associated equipment, such that comparisons could be made between the various parallel, antiparallel, and perpendicular orientations thereby made possible. The work with this is not yet complete, but already has confirmed the symmetry and usefulness postulated for the perpendicular arrangement and had confirmed the asymmetry and sensitivity to alignment of the parallel and anti-parallel mismatched double crystal spectrometer arrangements.

Fig. 5 shows the appearance of reflections obtained with the direct source and with the perpendicular monochromator arrangement using the source at various take-off angles and at both plus and minus two theta in some instances. This illustration was first shown at the Gatlinburg ACA meeting in June 1965 (Furnas & Beard, 1965; Beard, 1968).

Fig. 6 was shown by Mr D.W.Beard at the first meeting of the Italian Association of Crystallography in Perugia, Italy in January 1968 (Beard, 1968) and illustrates the striking differences between the appearance as recorded at the detector of reflections from a tiny beryllium acetate crystal specimen when illuminated: *A*, by the direct beam; *B*, by a quartz monochromator; *C*, by a highly oriented graphite monochromator of 0·52° mosaicity (full width at half-maximum intensity); and *D*, as in *C* but 1·0° mosaicity.

From the sizes of the reflections shown in Fig. 6 *C* and *D*, together with other ways in which these mosaic monochromators act, we can say that it is *as though* the mosaic monochromator were a doubly bent crystal of appropriate radius for use with whatever radiation you desire and of aperture equal to its mosaic spread. Thus it is indeed possible that if you were to use a very fine focus X-ray tube (and because this has no affect upon the mosaic spread of the graphite monochromator) you may be able to observe a reflection from the specimen crystal as much as ten times the intensity with the monochromator as when viewing that particular X-ray source directly. If the X-ray source itself is larger, then the difference in solid angle which the source subtends at the specimen compared to the mosaicity of the monochromator is less, hence the gain will be less. It is a function of what the particular experiment is which you are doing as to whether the *gain* is worthwhile or whether a different X-ray optical situation in which the gain is appreciably less than unity would be better.

These are some of the kinds of questions in which I feel we have great need for investigation.

We've had discussions regarding the uniformity of irradiation of the specimen. It must concern not only the intensity distribution in the specimen volume but also the spectral distribution and the directiveness or diffuseness of that spectral intensity distribution.

In 1959 at Stockholm I described a technique (Furnas, 1959) by which all four quantities can be determined, *i.e.* spatial position, relative intensity, spectral content *and* direction. – To the best of my knowledge, no one has yet performed the experiment for a real case. I had performed portions sufficient to prove its validity, but never completed the device to permit its complete operation.

The suggestions for enormous on-line computers to handle the correction problems seem quite at odds

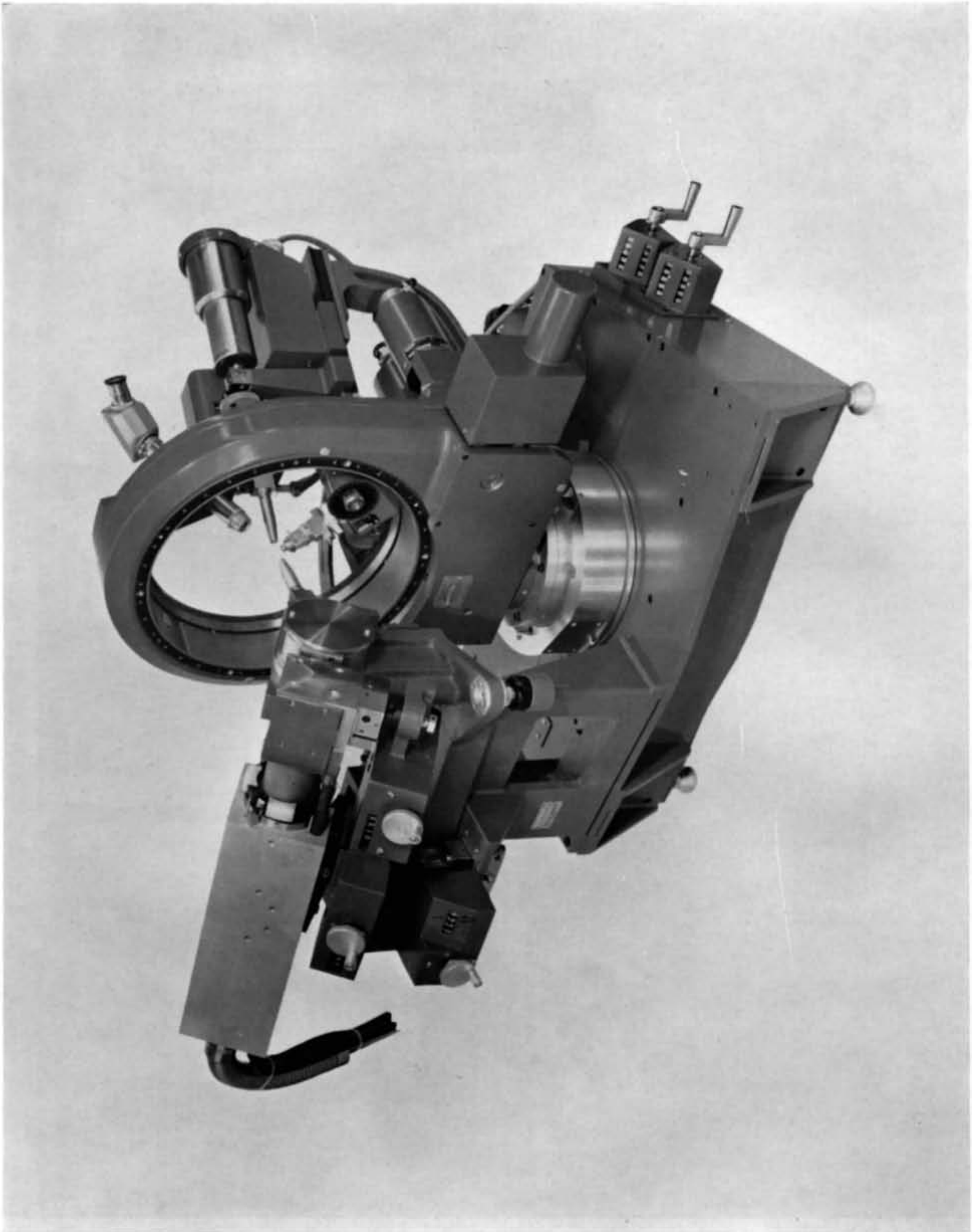

Fig. 3. The perpendicular monochromator arrangement with a four-circle diffractometer.

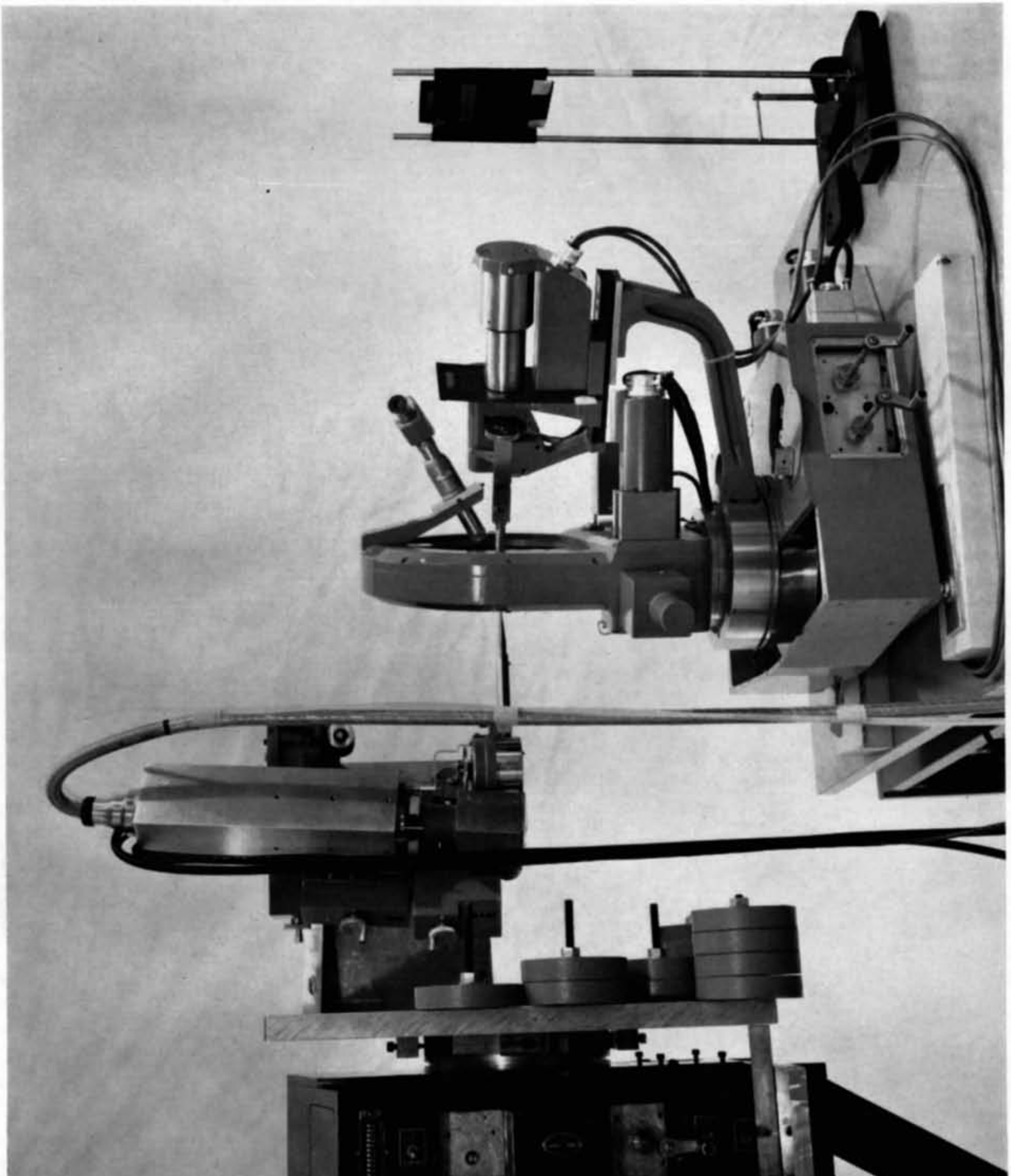

Fig. 4. Rotatable mount for changing the relative incident beam – specimen orientation.

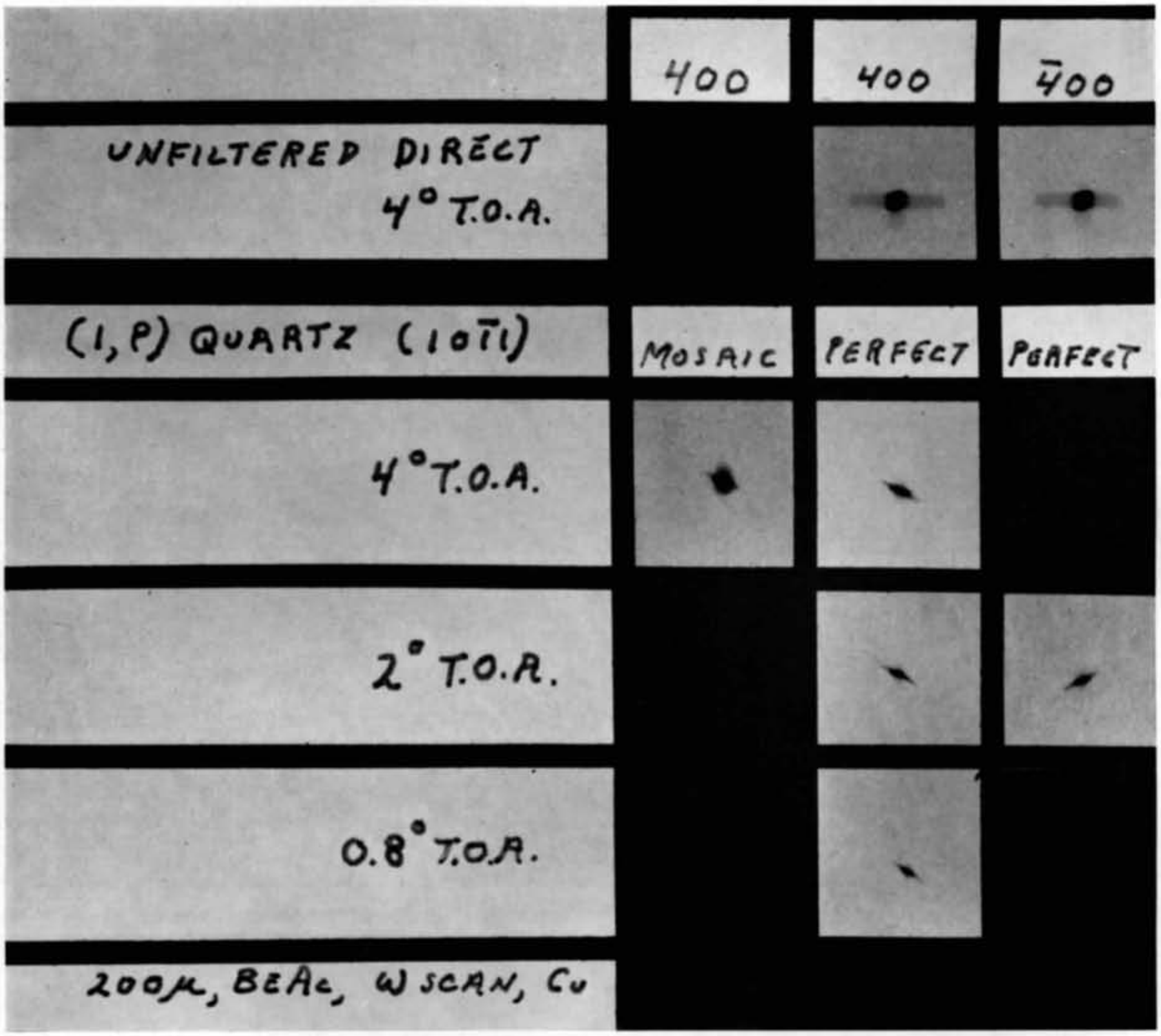

Fig. 5. Diffracted beam shapes depend on incident beam characteristics – note diagonal spectra and symmetry with perpendicular monochromator.

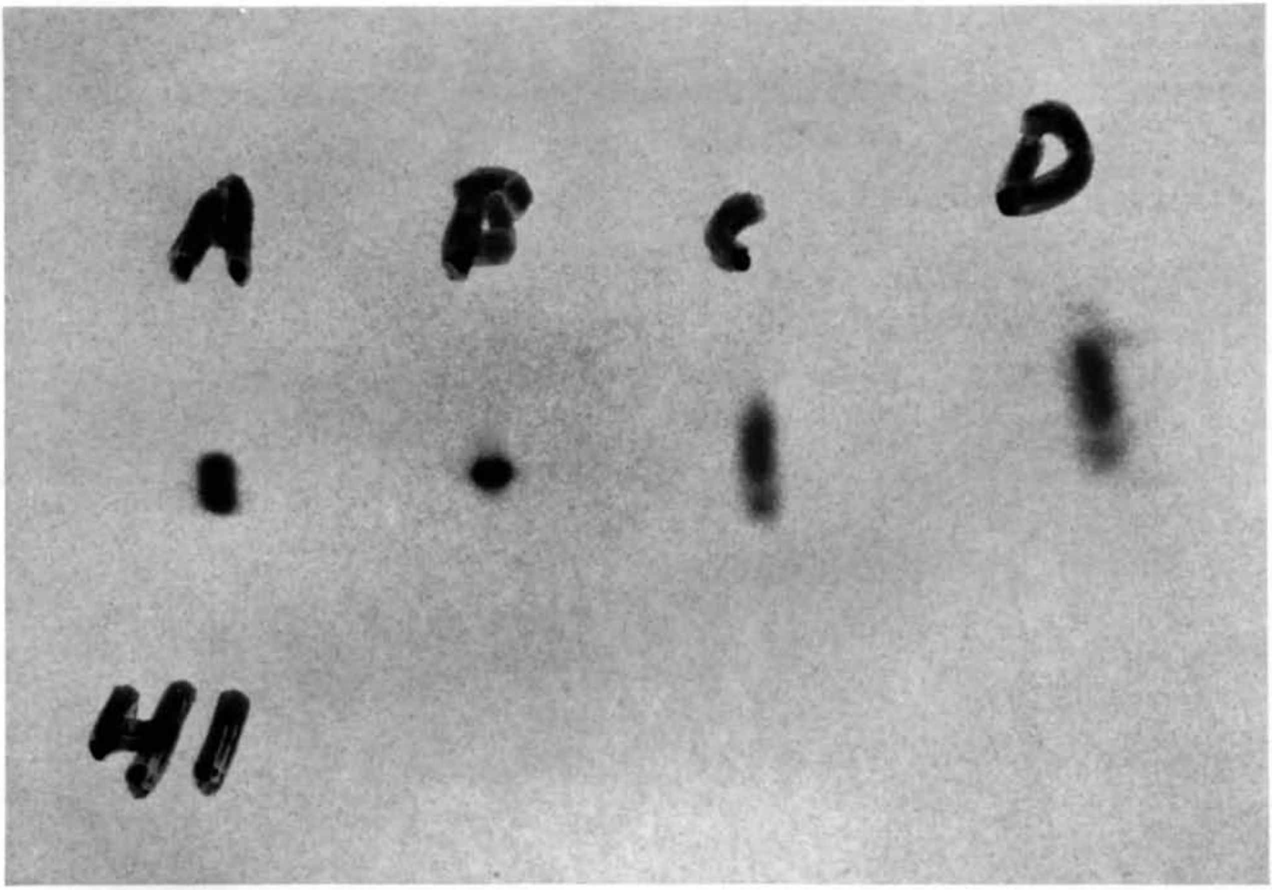

Fig. 6. Shape and size characteristics of reflections using: *A*, direct beam; *B*, quartz monochromator; *C*, graphite monochromator (0·52 degree FWHM); *D*, graphite monochromator (1·0 degree FWHM).

with the economics of the value of the results, *certainly* in view of the fact that we do not currently know what to correct and how.

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DISCUSSION

JEFFREY: Have you any evidence or comment on how the intensity distribution on the target might be different for different wavelengths?

FURNAS: It arises from the fact that characteristic X-rays are generated close to the surface and harder radiation beneath. Therefore absorption, polycrystallinity, surface roughness, *etc.* all will have different effects at different wavelengths as one changes from high to low take-off angles. An idea of the effect can be gained by comparing photographs taken at high voltages and at low voltages just sufficient to excite the characteristic radiation. They rarely agree when the resolution is sufficient to resolve the individual windings of the filament.

LADELL: Some combinations of a monochromator crystal and a specimen crystal may constitute a two-crystal spectrometer situation. In the case of a well-centered specimen for single-crystal structure data there arise other questions regarding resolution and the location of slits associated with problems of angular divergence of beams.

FURNAS: The role of the slit system in a monochromator crystal-specimen crystal assembly for the measurement of intensity is largely of secondary importance, being merely to define outer limits to beams and prevent excessive scatter into the laboratory. Angular divergences of single wavelengths are determined by the monochromator crystal whereas total wavelength spread and total angular divergences are determined by the dimensions of the specimen crystal and the size of the real or effective source – and, of course, the distances separating these items.

HOPPE: (1) If one is concerned about differences in profile of the primary beam due to different wavelengths then it is preferable to use lower voltages.

(2) A photograph is certainly best to show what a focal spot looks like.

(3) The chief reason for self-checking procedures during data collection is to see if something catastrophic happens to the crystal.

(4) Regarding the cost, I wholeheartedly agree that it is a problem, for on one structure on which I reported yesterday, one cycle of refinement took eight hours of 7090 time.

MATHIESON: Dr Furnas, in introducing a 90° rotation in the mutual relation of the monochromator and the specimen crystals, has added a new dimension to the Compton–Allison two-crystal spectrometer. It is one which definitely requires much investigation and should prove most useful. [See here paper by S. Chandrasekhar and also Mathieson, *Rev. Sci. Instrum.* (December 1968) **39**].