

By observing the reflexion of the light at a distance of several meters (we used a mark on the laboratory wall) one can readily achieve adjustment to within 0·05°. We could improve on this but our standard goniometer head did not allow us to make adjustments of less than 0·05°.

This use of the laser for alignment can also be adapted to crystal cutting equipment (alignment of a crystal face parallel to the circular saw). Accurate transfer of a crystal from the X-ray unit to the cutting equipment is facilitated. Finally, translation of the point of reflexion along the crystal face followed by rotation of the crystal provides a rapid means of checking the flatness of the face.

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(Received 12 July 1976;
accepted 3 August 1976)

J. Appl. Cryst. (1976), 9, 511

A source of harmonic-free X-rays

Crystals of thiourea dioxide exhibit a number of reflexions which are essentially free of harmonic radiation because they have intense first orders and negligible higher orders.

It is sometimes useful to have a beam of X-rays which is intrinsically free of harmonic radiation and to produce such a beam by X-ray diffraction, a crystal is required with a strong first-order reflexion and higher orders of negligible reflecting power. A survey of published structure factor tables shows that this is a fairly uncommon occurrence. However, for thiourea dioxide (Sullivan & Hargreaves, 1962), there appear to be seven reflexions that satisfy this stringent condition: 011, 121, 131, 141, 151, 140 and 301.

The thiourea cell parameters were redetermined on a Picker diffractometer with Cu K α radiation and the results obtained compare well with those of Hargreaves & Sullivan (given in parentheses): $a = 10\cdot116 \pm 3(10\cdot13)$, $b = 10\cdot666 \pm 3(10\cdot65)$, $c = 3\cdot920 \pm 2(3\cdot92)$ Å.

The intensities of the 011 series of reflexions were remeasured with Mo K α radiation and the results are given in Table 1. Assuming the intensity of bremsstrahlung radiation always to be less than

5% of the characteristic line intensity, the 011 diffracted beam will contain less than 0·02% harmonic content.

Table 1. *Integrated intensities of the thiourea dioxide Okk series of reflexions*

<i>hkl</i>	Integrated intensities
011	3085 000
022	21 715
033	2 780
044	3 061
055	6
066	0
077	0
088	0

Thiourea is easily obtainable, crystallizes well from water, appears to be chemically stable and is not readily damaged by X-irradiation. It has a pronounced (100) cleavage plane and can be easily cut in any direction parallel to [010]. Crystals of this compound should therefore provide a simple means of producing harmonic-free X-ray beams.

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(Received 22 June 1976;
accepted 30 July 1976)

Reference

Sullivan, R. A. L. & Hargreaves, A. (1962). *Acta Cryst.* **15**, 675–682.

Meeting Report

J. Appl. Cryst. (1976), 9, 511

Institute of Physics Crystallography Group Meeting

Aberdeen, 13–15 April 1976

Once again the Crystallography Group decided to run its spring meeting with no specific title in order to encourage contributions on any aspect of crystallography. Papers devoted to 'Advanced Techniques' were particularly requested and these amounted to about half the final contributions. Nineteen papers were

presented during a poster session. These were mainly concerned with structural determinations which are ideally suited to this style of presentation. The allotted two-hour session was substantially overrun as participants informally discussed detailed results with the authors.

The eighteen papers presented orally commenced with Baker (Harwell) describing his generalized approach to X-ray diffraction. As he pointed out, the basis of most diffraction experiments is the accurate measurement of the variation of X-ray intensity with angle. His system consists of a single base unit on which various attachments can be rigidly clamped to obtain the required experimental geometry. The whole is computer controlled, all necessary movements being made by stepping motors.

Glazer (Cambridge) described how synchrotron radiation can be used for a variety of X-ray experiments. Direct comparison between experiments using a conventional X-ray source and experiments using synchrotron radiation is meaningless because of the widely different source outputs. Synchrotron radiation is most suited to energy-dispersive techniques as the beam is always highly parallel. The resulting fixed specimen position greatly facilitates experiments involving a variable specimen environment. The intensity available is extremely high, which can be exploited in fast X-ray topography and the study of biological materials which rapidly deteriorate.

Swindells (Liverpool) described how a focused electron beam of less than 5 μm diameter can be used to generate Kossel Patterns. With this technique it is possible to find the orientation, structure and plane spacing of each crystallite of a multiphase metallurgical sample.

Three other papers dealt with specific experimental techniques. A group from Aberdeen described their experience with a hot stage used with a powder diffractometer. Johnson (British Steel) reviewed the use of focusing cameras – the ensuing discussion indicated that this is very much more of an art than a science. Faruqi (Cambridge) described his experience with position-sensitive detectors to study short-lived muscle fibres.

The remainder of the papers dealt with either materials investigations or methods of processing diffraction data. The range of materials studied was wide, as was the range of techniques used to study them. Bilsby and Ferguson (UKAEA) studied the corrosion films on zircaloy using X-ray diffraction, electron diffraction and Auger spectroscopy. Halliwell (Post Office) describes how multi-epitaxic gallium alu-

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minium arsenide layers could be assessed by using Lang topography and double-crystal rocking curves. Other materials studied were polyethylene, barium titanate, graphite and the Y-Si-O-N and Si-Al-O-N systems.

In the group of papers related to data analysis, Reid (Aberdeen) gave a very clear account of how temperature diffuse scattering arises and how it can be recognized. He gave calculations to show its variation with temperature and order of reflexion for the sodium chloride structure. Wilson (Birmingham) gave a physical interpretation of the various methods currently used for calculating the residual, R , for a structure. Gilmore (Glasgow) described the advantages of using quartets rather than triplets when solving structures with space group $\bar{P}1$ by direct methods. Lawrence (St. Andrews) described how to determine absolute structure factors when crystals large compared to the incident beam are available.

Murray-Rust (Stirling) gave the final paper in this most varied and stimulating conference. He suggested that, rather than use the classical scientific methods of developing a theory followed by collecting data to support it, crystallographers could well use sociological methods. This would entail extracting data already available, for instance from the Data File for organic compounds at Cambridge, searching for correlations and finally developing theories to account for the observations.

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(Received 7 May 1976;
accepted 11 June 1976)

Crystallographers

This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England).

Professor Dorothy Hodgkin, Wolfson Research Professor of the Royal Society and Immediate Past President of the International Union of Crystallography, has been elected President of the British Association for the Advancement of Science for the period of one year from September 1977.

Dr S. Iijima and Professor J. M. Cowley, both of Arizona State University, Tempe, U.S.A. have been named recipients of the Bertram E. Warren Award in diffraction physics, for the development of techniques for the direct imaging of crystal structure atom configurations through the use of high-resolution electron microscopy. This award is presented by the American Crystallographic Association under the sponsorship of IBM.

International Union of Crystallography *Structure Reports*

Volume 40A of *Structure Reports*, covering the literature for metals and inorganic compounds for 1974 (viii + 342 pages), has recently been published at a price of 130 Netherlands guilders.

A 60-Year *Structure Index*, covering the period 1913–1973, has been compiled and is now being published. It is divided into two sections: Section A. *Metals and Inorganic Compounds*, and Section B. *Organic and Organometallic Compounds*. Either section may be purchased separately. The complete indexes have been prepared by computer and have been printed as computer-produced listings with upper and lower case letters. Section A contains a metals classified index, a metals structure-type index, an inorganic compounds index and a mineral name index, each of which includes names of materials, formulae and references. Section B contains an index based on a chemical classification (and lists name and formula), a formula index and a transition-metals index. Section A consists of $x + 229$ pages and costs 80 Netherlands guilders; Section B of $x + 437$ pages and costs 190 Netherlands guilders.

A separate cumulative index covering the whole published series of *Strukturbericht* (Volumes 1–7; 1913–1939) is also being published. It is a reorganized and expanded version of the original individual volume indexes. It makes information readily available on all the fundamental crystal structures which were determined in that period. It consists of $vi + 91$ pages of subject (English translation), formula and author indexes, and costs 50 Netherlands guilders.

Orders for any of these publications may be placed direct with the publisher, Bohn, Scheltema & Holkema (formerly Oosthoek, Scheltema & Holkema), Emma-laan 27, Utrecht, The Netherlands, with Polycrystal Book Service, P.O. Box 11567, Pittsburgh, Pa. 15238, U.S.A. or with any bookseller.

Report of the Executive Committee for 1975

The Report of the Executive Committee for 1975 has been published in *Acta Crystallographica*, Section A [*Acta Cryst.* (1976). A32, 1019–1033]. It reports as usual on the meetings and publications of the Union, the work of its Commissions, and the work of bodies not belonging to the Union but on which the Union is represented.

Prices of *Acta Crystallographica* and *Journal of Applied Crystallography*

The Executive Committee of the International Union of Crystallography has found it necessary to increase the yearly subscription rates and also the prices of back numbers for *Acta Crystallographica* and *Journal of Applied Crystallography* as from 1 January 1977.

Acta Crystallographica

The following rates will apply for Volumes A33 and B33 (1977). All subscription rates are fixed in Danish kroner, and the U.S. dollar equivalents given below are subject to exchange-rate fluctuations.

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The reduced-rate subscriptions are ordinarily only available to members of recognized scientific societies, and applications must be accompanied by a written undertaking that the journal is for the personal use of the subscriber and will not be made available to libraries, institutions, etc. These conditions also apply to persons wishing to order back numbers at the reduced rates.