the additional system has the same symmetry as the original one. The many-beam systems studied by Ploc & Miller will therefore be degenerate at some non-zero misorientation, as is illustrated in Fig. 1 for the Al 111 systematic row.

In the first place this explains why Ploc & Miller found only a minimizing of the separation between the two branches, since their computations were run under the exact Bragg condition. It also accounts for the anomalous behaviour of the excitation amplitudes they showed: this must be similar to the behaviour in the correct systematic case for a small misorientation, as illustrated in Fig. 2. The proof of the latter assertion requires a renormalized perturbation calculation and will be given in a later paper on the influence of non-systematic reflexions. The latter are expected to cause the same qualitative effects as inadequate higher-order systematics since in both cases the symmetry of the dynamical system is broken. We may thus conclude that the results of Ploc & Miller are irrelevant for the purely linear C.V.E.

The use of an inadequate many-beam system for numerical calculations on the C.V.E. is not unique in the literature. Usually a very large number of reflexions are used so that the errors introduced become negligible [see, for example, Metherell & Fisher (1969)]. Practically correct results are then obtained, however, only at the expense of a large computer time. The problem we have commented on here illustrates, moreover, the danger of drawing conclusions from numerical calculations alone without a thorough analytical understanding of a problem to guide them.

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A test on the statistics of derived intensities*.

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Variances of X-ray reflexions calculated with the procedure as proposed by McCandlish, Stout & Andrews [*Acta Cryst.* (1975), A**31**, 245–249] have been tested against variances determined in an independent way. A satisfying agreement is obtained.

On theoretical grounds one expects the variance σ^2 of an X-ray reflexion to be equal to the total number of counts T:

$$\sigma^2(I) = T. \tag{1}$$

I represents the number of net counts. As is well known the variance derived in this way does not represent sufficiently all errors. A term proportional to I^2 is often included:

$$\sigma^2(I) = T + F^2 I^2. \tag{2}$$

Several rationalizations have been given (McCandlish, Stout & Andrews, 1975).

The factor F is commonly chosen between 1×10^{-2} and 5×10^{-2} in an empirical way. To give some background to equation (2) a discussion of the variance has been given by McCandlish *et al.* (1975). They considered instrumental instability and data scaling. The following formula was derived:

$$\sigma^2(I) = K^2 T + S^2(K) I_o^2 + K^2 P^2 I_o^2 \tag{3}$$

where K is the scaling factor (or function), I_o the observed net intensity, I the real net intensity, $S^2(K)$ the variance of K and P the instability factor which can be estimated from reference reflexions.

A P value of 4×10^{-3} to 8×10^{-3} has been reported by McCandlish *et al.* (1975) for their card-controlled Picker diffractometer. To test this formula an analysis of a recently measured X-ray data set of pyrazine (de With, Harkema & Feil, 1976) was carried out. Because in this data set each independent reflexion has been measured approximately seven times, (symmetry-related ones and partial repetition), it was possible to calculate for each reflexion an external variance. On the other hand, an estimate of the contribution of instrumental instability and scaling procedure to the variance could be made, due to repeated measurement of three reference reflexions.

The variance estimated with equation (1) (counting statistics only) was tested against the external variance using the χ^2 test at a 97·5% confidence level. Curve A in the figure shows the ratio R of the experimental χ^2 value to the expected χ^2 value as a function of $\sin(\theta)/\lambda$. The curve presented is a smoothed one, representing average values. Each average contained reflexions from equal parts of reciprocal space (as covered by the experiment), a part being roughly equivalent to 20 reflexions (the behaviour of the curve was largely independent of the exact number of reflexions in each part). This means that a significant difference is expressed in Fig. 1 as a ratio greater than one. As can be seen from the plot, differences are significant upto $\sin(\theta)/\lambda = 0{\cdot}75$ Å^{-1}. This indicates once again that counting statistics alone do not represent properly the variance of a reflexion.

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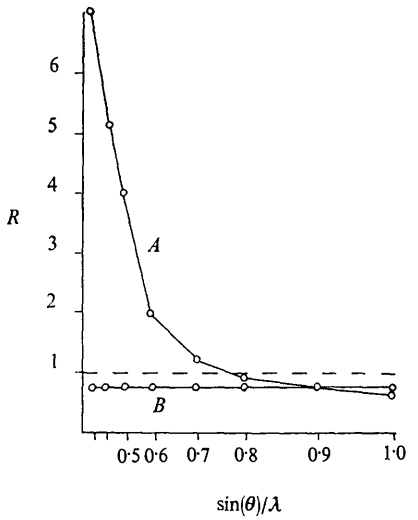

Fig. 1. The ratio R of the experimental χ^2 value to the expected value as a function of sin $(\theta)/\lambda$. Curve A: calculated from counting statistics alone [equation (1)]. Curve B: calculated from the procedure as proposed by McCandlish *et al.* (1975) [equation (3)].

The test was also applied to the variance as estimated with equation (3). P was calculated from the three reference reflexions ($P1 = 2{\cdot}1 \times 10^{-3}$, $P2 = 3{\cdot}3 \times 10^{-3}$, $P3 = 2{\cdot}9 \times 10^{-3}$) resulting in an average P value of $2{\cdot}8 \times 10^{-3}$ (Philips PW1100 computer-controlled diffractometer). The variance of K showed no marked systematic time dependence, probably because of the highly consistent behaviour of the reference reflexions. Therefore for both K and $S^2(K)$ average values were used [$K = 1{\cdot}22$, $S^2(K) = 4{\cdot}9 \times 10^{-4}$]. In this case the terms $S^2(K)I_o^2$ and $K^2P^2I_o^2$ can be taken together. The square root of $S^2(K) + K^2P^2$ equals $2{\cdot}2 \times 10^{-2}$ and is directly comparable with F, equation (2). Using the same procedure as before curve B in Fig. 1 was obtained. This time no significant differences exist. Hence we may conclude that the procedure of McCandlish *et al.* is, at least in this case, a satisfactory one.

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International Union of Crystallography

Commission on Electron Diffraction.

Guide for the Publication of Experimental Gas-Phase Electron Diffraction Data and Derived Structural Results in the Primary Literature*

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This report contains general recommendations for the guidance of authors, referees, and editors on the reporting of electron diffraction data and derived structures. They are intended to facilitate reliable evaluation, ease of comparison with other data, and the retrieval of information if later reanalysis becomes desirable in the light of new theories or experiments.

Introduction

This report is concerned with the presentation of structural investigations by electron diffraction. Its aim is to make results obtained by specialists more accessible to those in other disciplines and, at the same time, to increase the potential value of the original data to other specialists if subsequent events warrant reinvestigation. The needs of compilers and correlators of information will also be benefited by attention to these considerations. Only if enough information is provided to allow readers to appraise the precision and accuracy of the work, and only if reasonably uniform standards of reporting the results are adhered to, can all ends be met.

This report is an abbreviated version of a document approved by the Commission on Electron Diffraction of the International Union of Crystallography in August, 1975. For its general recommendations the original document quoted extensively from the *Guide for Publication of Experimental Data and Derived Numerical Results in the Primary Literature* prepared for CODATA and UNESCO in 1973 by the CODATA Task Group on Publication in the Primary Literature (1973). The present report concentrates on specialized problems encountered in the field of gas-phase electron diffraction, certain aspects of which have been referred to in review papers in the field (Akishin, Rambidi & Spiridonov, 1967; Bartell, 1971; Bastiansen, Seip & Boggs, 1971; Bauer, 1970; Beagley, 1973; Davis, 1971; Haaland, Vilkov, Khaikin, Yokozeki & Bauer, 1975; Hilderbrandt & Bonham, 1971; Karle, 1973; Kuchitsu, 1972*a*, *b*; Robiette, 1973; Seip, 1973). Literature citations are illustrative, not exhaustive.

While an adequate documentation of experiment and interpretation is vital, so also, in the avalanche of scientific literature we must contend with, is brevity and conciseness. Possible ways to achieve both ends are as follows. It would be desirable to develop a compact style of reporting essential details that vary from analysis to analysis. Standard equipment and procedures in a given laboratory that have been described clearly in readily available journals or accessible depository services may be documented simply by citing the appropriate references. Workers in every laboratory have an obligation to provide this information, as outlined in the following sections and to revise it every few years when substantial changes are made. Special procedures and certain data that are important for a critical evaluation of results but not of general interest to readers should be summarized and placed in a suitable depository service or published as microfilm together with the article.

More and more highly specialized computer routines are being used to process data, to convert it to molecular parameters, to compute the effects of a host of influences such as electron density shifts, distortions of diffracted waves, molecular vibrations, *etc.*, and to interpret derived structures in terms of quantum-chemical or other models. References to important computer packages employed and their sources should be given.

Structural investigations by gas-phase electron diffraction differ so much in complexity and in aim that it is impractical to recommend rigid rules for the reporting of procedures and presentation of results. Investigations in which low precision suffices need not be documented as minutely as those in which high precision is claimed. In the following are presented recommendations intended to be helpful in the preparation of a full paper. This guide may not fit all cases, and future developments may necessitate modifications. However, it is our hope that authors will deviate from the recommendations only after careful consideration.

I. Experimental apparatus and procedures

An adequate description of the experimental procedures used to obtain the numerical results should be made available. The major points to be considered are:

* This report is based on a draft written in 1973 by the Gas-Diffraction subcommittee of the IUCr Commission on Electron Diffraction in consultation with workers in a majority of the existing laboratories of electron diffraction. The present version incorporates suggestions received during discussions of the *Guide* in scheduled open sessions at the Austin Symposium on Molecular Structure, Austin, Texas, March, 1974; the Second European Crystallographic Meeting in Keszthely, Hungary, August, 1974; and the Tenth International Congress of Crystallography in Amsterdam, August, 1975; and by correspondence from interested IUCr members.