

Systematic and Random Powder Diffractometer Errors Relevant to Phase Identification

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Abstract

A variety of systematic and random errors affect the "d" values experimentally obtained from a powder diffractometer. Fortunately, not all of these bear significantly on the use of a set of "d" spacings for the purpose of phase identification. This paper reviews and reports on an experimental study of the major errors, and attempts to order them with those most affecting phase identification near the top.

Introduction

The X-ray powder diffractometer is employed for a multitude of purposes. Of these, phase identification is among the more common. Any analytical tool has associated with it many sources of errors, which range from those physically inherent in the analytical technique through instrumental aberrations and alignment, data collection and analysis procedures. Frequently, when an instrument is capable of being employed in a variety of ways, the impact of errors varies according to the function performed. Such is the case with the powder diffractometer, and thus, when we began to consider writing a search/match phase identification program for a minicomputer, it seemed prudent to review the various systematic and random errors affecting successful phase identification and attempt to order them with those most influential to phase identification at the top. If necessary, the most important of these might be explicitly considered in the phase identification software, while the less important ones might be compensated for either theoretically, through calibration, or simply ignored if appropriate. This paper presents the results of our work.

Theoretical Versus Experimental Calibration Curves

The first step in evaluating the relative importance of the various systematic errors is to review those which have been studied theoretically in the past^{1,2,3}. In order to compare the sign and magnitude of the various errors, we will present a series of figures all on the same scale so that the eye does not have to recalibrate itself in order to compare them. As a result of this approach, some of the curves may be too small to see clearly. However, unless the largest errors are first controlled, the details of the smaller errors are clearly irrelevant.

In Figure 1 the calculated shift from the ideal 2θ position due to axial divergence (AD) and flat specimen (FS) errors is displayed. The flat specimen curve includes the effect of a theta compensating slit which is normally part of Philips instruments. Both errors shift lines toward low angles below about $100^\circ 2\theta$, the important region for phase identification. Note that the axial divergence, according to Pike's formula⁴ diverges at low 2θ .

Figure 2 shows the effect of specimen transparency. Typically inorganic samples have linear absorption coefficients greater than 50 cm^{-1} , as the absorption coefficient increases, the error goes to zero. For organic specimens, however, very substantial shifts may be observed and these shifts are maximum at $90^\circ 2\theta$.

If we add these three errors together, taking quartz as a typical inorganic specimen, we obtain the total inherent error seen in Figure 3. Over the range 20 – $100^\circ 2\theta$ it will be apparent

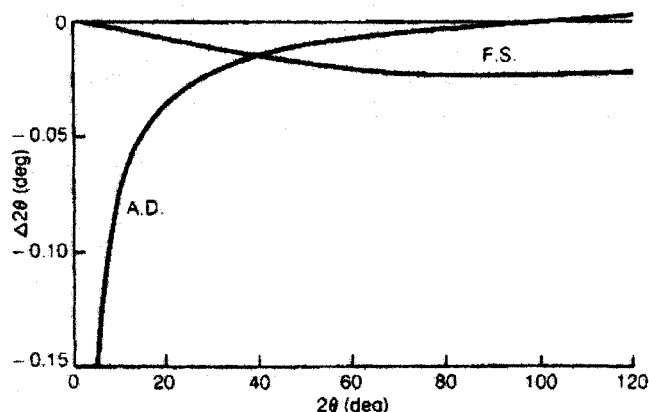


Figure 1. The calculated shift, c.g., (center of gravity) from the ideal 2θ position, as a result of axial divergence (AD) and flat specimen (FS) errors. The (FS) curve includes the effect of a theta compensating slit.

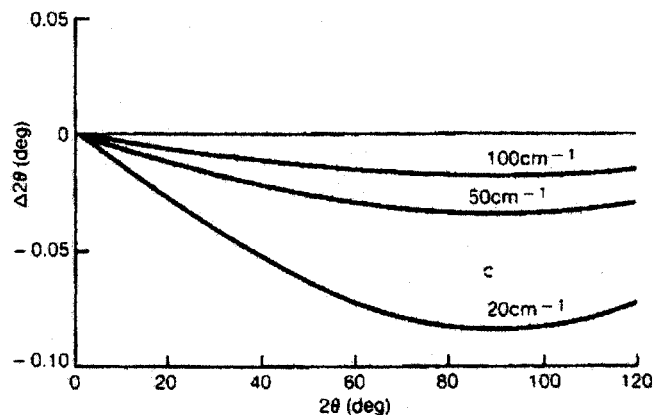


Figure 2. The effect of specimen transparency (c.g. shifts). Substantial shifts may be observed for organic specimens, where linear coefficient is small.

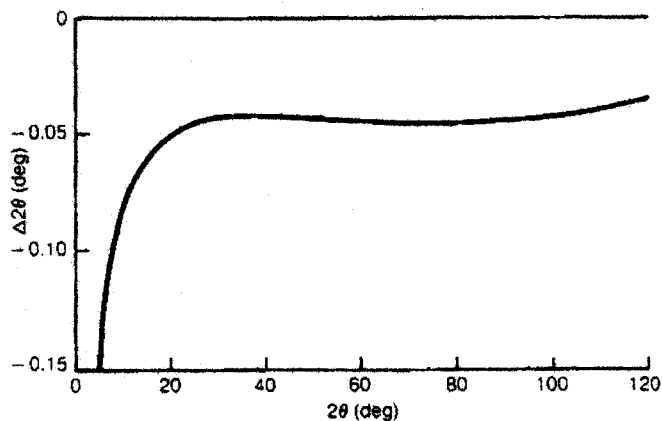


Figure 3. Total systematic error calculated for quartz.

that there is a systematic difference of about $-0.05^\circ 2\theta$. Such an offset could easily be mistaken for a zero angle error.

To see if this constant offset could be observed experimentally, we carefully measured quartz ($\alpha\text{-SiO}_2$) using a Philips Automated Powder Diffractometer⁷. Instead of the predicted shape, we observed that the data fell along a sloping

DELTA TWO-THETA VS. TWO-THETA

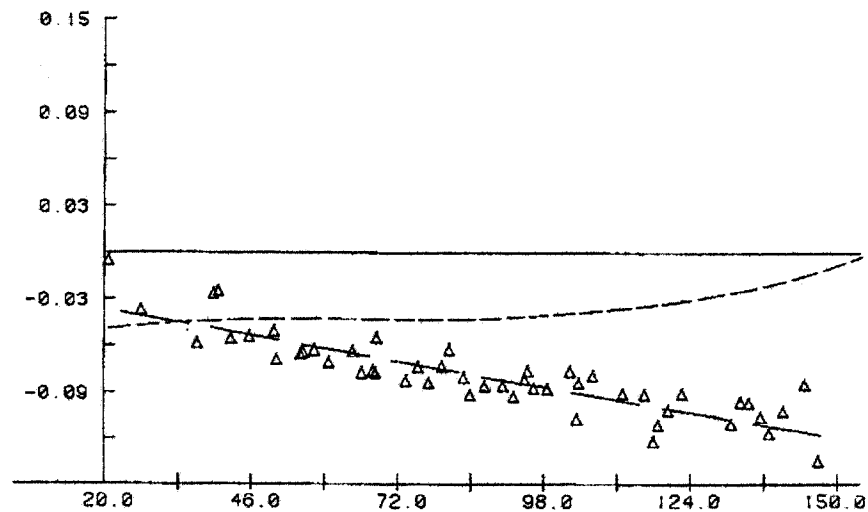


Figure 4. An experimental measurement of quartz indicates that the systematic error function does not agree with the theoretical prediction.

DELTA TWO-THETA VS. TWO-THETA

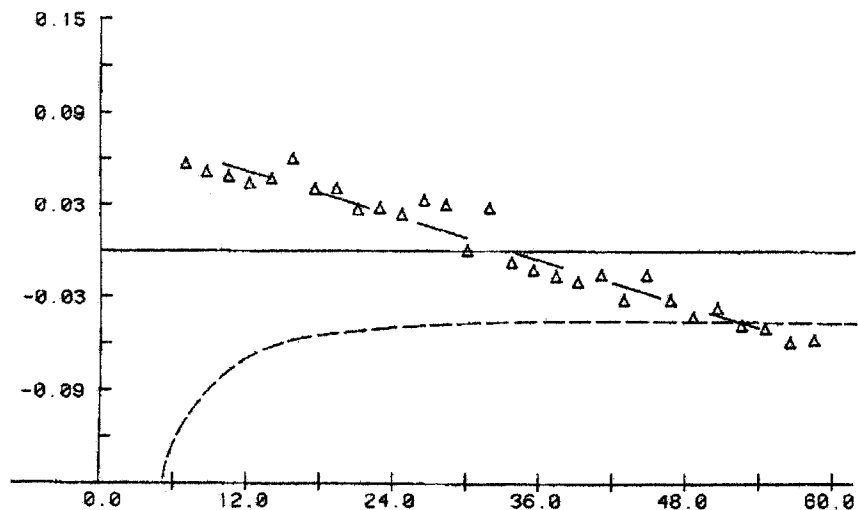


Figure 5. Observation with a lead stearate monolayer crystal, made to determine behavior of calibration made at low angles, showing similar disagreement with theoretical assumptions.

"calibration" line (Figure 4). To see the behavior of the calibration mode at low angles we used a lead stearate monolayer crystal and measured lines down to $7^\circ 2\theta$. Still the data fit a straight line as seen in Fig. 5. We observe that the values disagree in shape, magnitude and sign. Regarding these measurements we make the following observations.

First, it seems intuitively clear that there must be a problem with the Pike's axial divergence term⁴ at low angles since it involves cot and csc functions which become infinite as 2θ approaches zero. Infinite peak shifts are physically not possible. The infinities probably result from approximations made in the derivations which are not valid as 2θ approaches zero.

Second, we measure peak positions, not line centers-of-gravity (c.g.). Theoretically, c.g. shifts are easier to calculate than peak shifts and they have the nice property that they add algebraically, while peak shifts do not. This fact has long been known⁵ and is the reason c.g. measurements are often used for precision lattice determinations. However, experimentally, peak positions are more easily determined since one does not have to worry about how to cut off the profiles. Thus, from a practical point of view, we are more interested in the behavior of peak positions. Evidently the line asymmetry, which is a function of 2θ , causes the calibration curve of peak positions to develop a slope. Theoretical work in this area would certainly

be very useful to confirm this conjecture.

Third, the geometry of today's diffractometers is somewhat different from that for which Wilson, Pike and others derived their theoretical error functions. For example, the optics of today's diffractometers widens from 12mm at the divergence slit to 18mm at the receiving slit, whereas past theoretical work assumed a uniform geometry. Also today's diffractometers include theta-compensating slits and monochromators whose effects are not included in the integration limits.

Fourth, the contributions of non-geometrically related errors such as diffractometer alignment errors, etc., are not included in the theoretical calibration curves seen in Figures 4 and 5.

In order to investigate some of these possibilities as well as to help characterize relative sizes of errors, we undertook an experimental study of the commonly encountered systematic errors. This work is discussed in the next section.

Experimental Study of Errors in Modern Diffractometers

Most of the systematic errors affecting powder diffractometry have been studied theoretically to one degree or another⁶, and, as we already mentioned, the work generally gives quantitative results for center-of-gravity shifts rather than peak shifts. Our interests here are of a very practical nature — to establish calibration curves based on measurements of peak positions, to see if new diffractometer optics have introduced any significant changes in expected calibration curve shapes, and to see if the source or the differences in the curves of Figures 4 and 5 can be elucidated.

The equipment used consisted of a Philips wide range goniometer, an XRG-3100 generator, a fine focus copper anode tube at a take-off angle of 6°, a theta-compensating slit and a fixed wavelength monochromator. These components are part of a standard APD-3600 automated powder diffractometer⁷ which was used to collect and analyze that data. The data was taken at 40–45 kV, 40 mA.

The experimental procedure was to measure specific lines of a reference material with the diffractometer normally aligned, then to introduce one change in the instrument such as removing the primary collimator, and report the observed line shifts as a function of 2θ . The reference specimen was α -SiO₂ (Arkansas stone) which was surface ground and lapped to a flatness of $\sim 10 \mu\text{m}$. The method of measuring peak positions was to scan over (isolated) peaks in .01° steps, strip the α_2 using a Rachinger algorithm and then least squares fit the top 10% to a parabola. It should be pointed out that this method of studying errors "individually" is not clean since the errors frequently couple to one another, however, such second order effects are not important for purposes of this paper and they do not affect the conclusion drawn.

Figure 6 shows the effect of removing the primary Solier collimator. The shape of the curve does not resemble the theoretical axial divergence c.g. shift given by Pike. One would expect shifts toward lower instead of higher angles as we see here. Can peak vs. c.g. measurements be responsible for so much difference?

Figure 7 shows the effect of removing the secondary collimator. Now peak positions shift to lower angles as the axial divergence term would predict. The line drawn through the points is a least squares fit to the data points and not a theoretical prediction. The principle reason for using a secondary collimator is to decrease scattered background radiation, and it apparently does little to reduce axial divergence beyond that of the primary collimator.

Figure 8 shows the result of decreasing the width of the receiving slit from 18mm to 10mm. No effect is seen. This in-

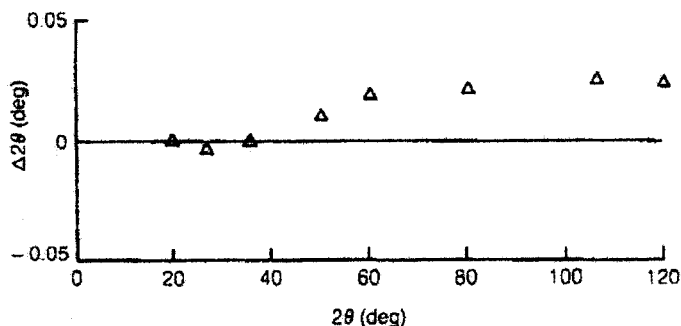


Figure 6. Effect on axial divergence of removing Solier slit.

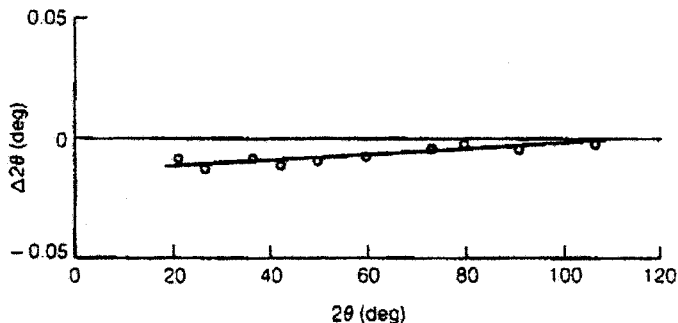


Figure 7. Effect on axial divergence of removing secondary collimator. Peak positions shift to lower angles, as predicted.

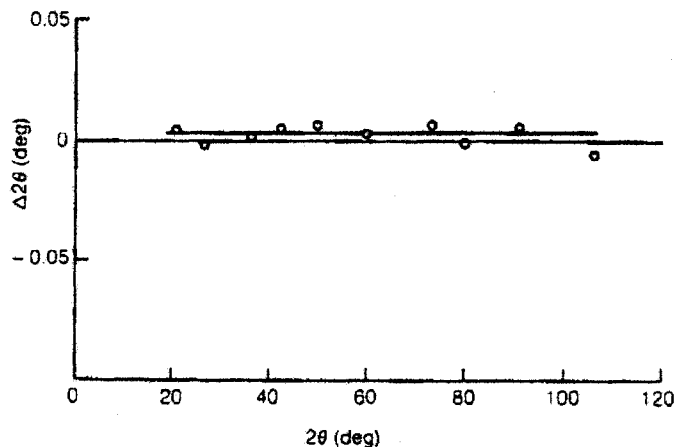


Figure 8. Decreasing width of the receiving slit from 18mm to 10mm shows no effect, indicating that axial divergence vignetting has been virtually eliminated with the widened optics of modern diffractometers.

dicates that axial divergence vignetting has been virtually eliminated with the widening optics of today's diffractometers.

Figure 9 demonstrates the effect of substantial 2:1 offsets. The lines here are only drawn to guide the eye through the data points. Negative offsets are seen to shift peak positions much more than positive offsets. Furthermore, negative offsets have the shape necessary to convert the theoretical curves of Figures 4 and 5 into the experimental ones. But when a diffractometer is mechanically aligned, 2:1 missettings of no more than 0.01–0.02° result. Thus the shifts associated with the error are negligible. Still, the fact that the negative offsets appear to become large at low 2θ warrants further investigation.

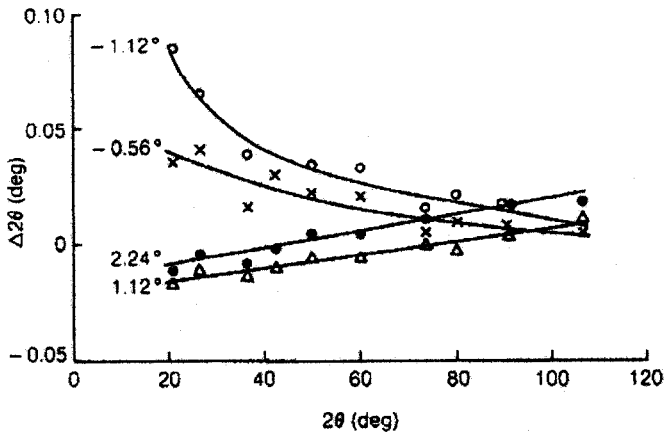


Figure 9. Effect of substantial 2:1 offsets. (Lines are drawn only to guide eye through the points.) Negative offsets shift peak positions much more than positive offsets.

Figure 10 shows the effect of changing the specimen to receiving slit distance by ± 2 mm. Maximum values encountered in practice are probably about ± 1 mm. Again, although the effect is not substantial, closer investigation at low 2θ values is warranted.

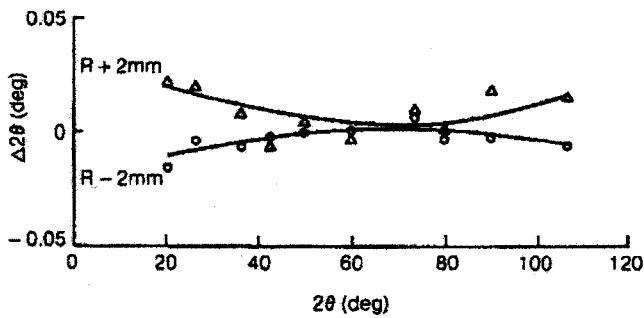


Figure 10. Effect of changing specimen-to-receiving distance by ± 2 mm.

The effect of decreasing the specimen illumination length from 15mm to 5mm is seen in Figure 11. The curve is the theoretical c.g. shift⁸ while the data, of course, are peak shifts. Even so, agreement is quite good.

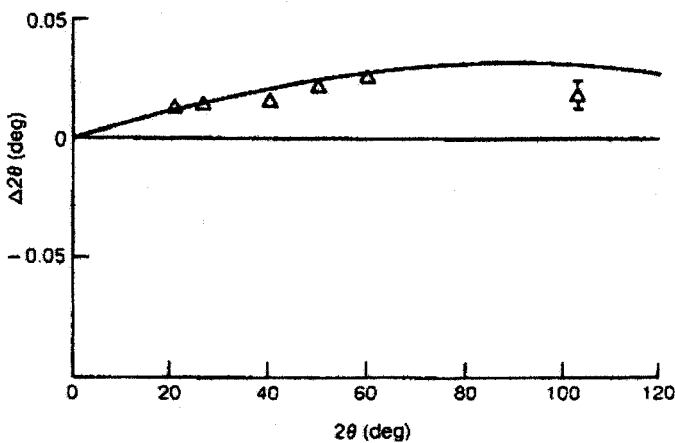


Figure 11. Effect of decreasing specimen illumination length from 15mm to 5mm.

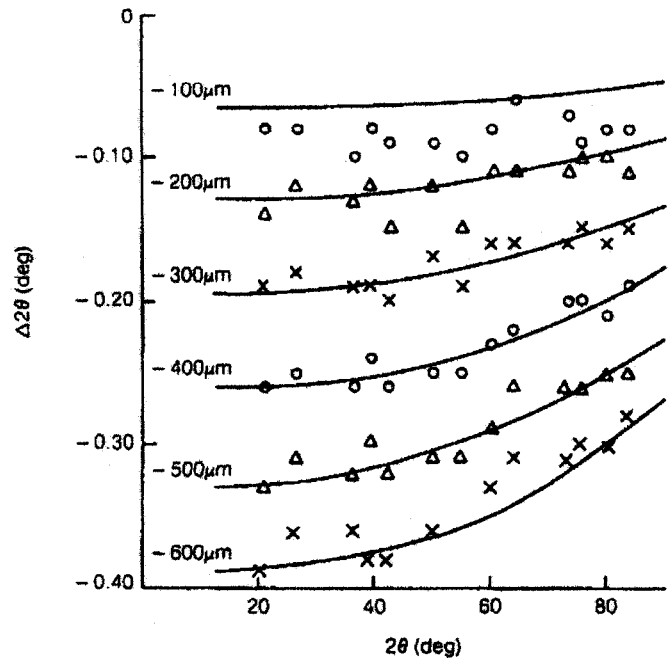


Figure 12. Specimen surface displacement error (drawn to a different scale to accommodate magnitude of error). Curves drawn are the theoretical c.g. predictions which are seen to agree well with peak data.

Specimen surface displacement error is seen in Figure 12. In this case the scales are different from those used before because the error is so large in comparison. The curves drawn are the theoretical c.g. predictions which are seen to agree very well with the peak data. In fact, it would appear that our $-100 \mu\text{m}$ displacement data were probably closer to $-140 \mu\text{m}$.

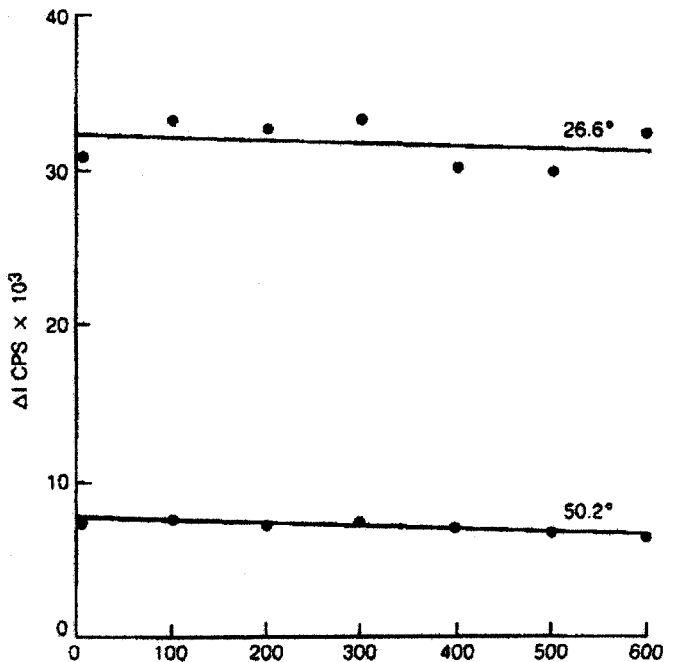


Figure 13. A plot of peak intensity change vs. displacement error shows, as expected, virtually no effect of one on the other.

We find in our own laboratories that about a fifth of the specimens we prepare have errors in excess of 100 μm , thus giving rise to very substantial peak shifts. We assume that our careful specimen preparation is no worse than that of other workers. This assumption seems to be confirmed by results obtained when our phase identification program, SANDMAN[®], analyzes data taken at other laboratories. SANDMAN allows a free parameter in the matching process to compensate for systematic line shifts. The parameter can be interpreted as a displacement error and gives us a way of monitoring that error when internal standards are not used. It appears that a 100 μm displacement error is not uncommon and we use it as a typical value.

Since displacement error has such a large effect we wondered if it causes any changes in the observed peak intensities. One would not expect any such effect, at least to first order. Data for two of the quartz lines seen in Figure 13 affirm that it does not.

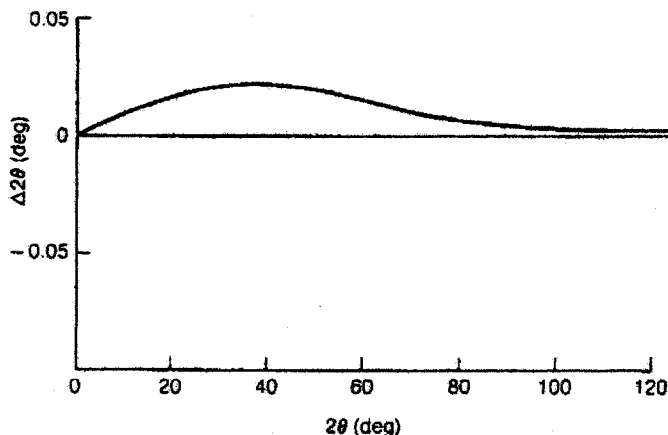


Figure 14. A plot of expected shift of peak position of alpha-1 due to presence of alpha-2 (if diffraction profiles are pure Lorentzians). The error is small and, with a simple alpha-2 stripping algorithm, can be reduced, essentially, to zero.

Two other errors, not measured experimentally, are included here for purposes of characterizing their size vis-a-vis other errors. Figure 14 shows the expected shift of the peak position of the alpha-1 due to the presence of the alpha-2, if the diffraction profiles were pure Lorentzians. The curve has a maximum around 40° 2 θ , the point at which alpha-1 and alpha-2 first become partially resolved. The error is small and with a very simple alpha-2 stripping algorithm can be reduced to essentially zero on this scale.

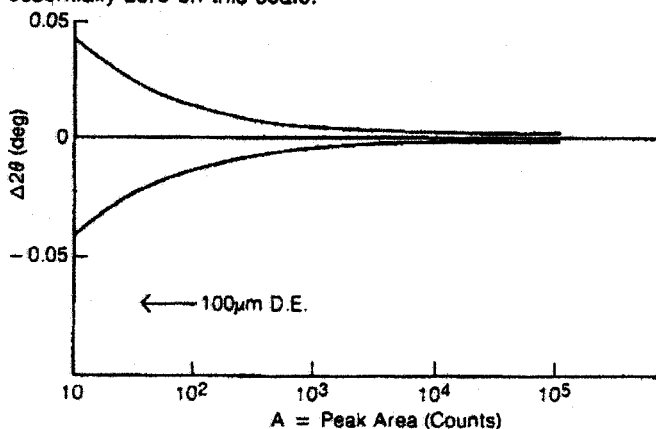


Figure 15. Effect of simple counting statistics on the location of Gaussian peak. Curves show that random error is inconsequential when peak contains more than 100 counts.

Figure 15 shows the effect of simple counting statistics on the location of a gaussian peak. The precision with which the peak of a gaussian distribution can be located is inversely proportional to the square root of the total number of counts observed (i.e., peak area). For a typical diffraction profile with a FWHM of 0.25°, it is seen that this random error is inconsequential when the peak contains more than about 100 counts.

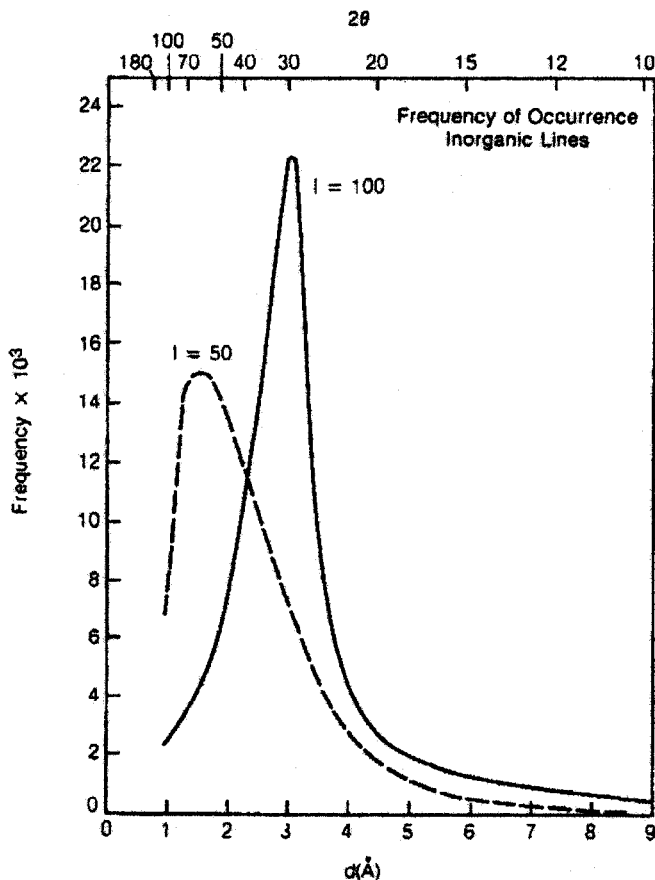
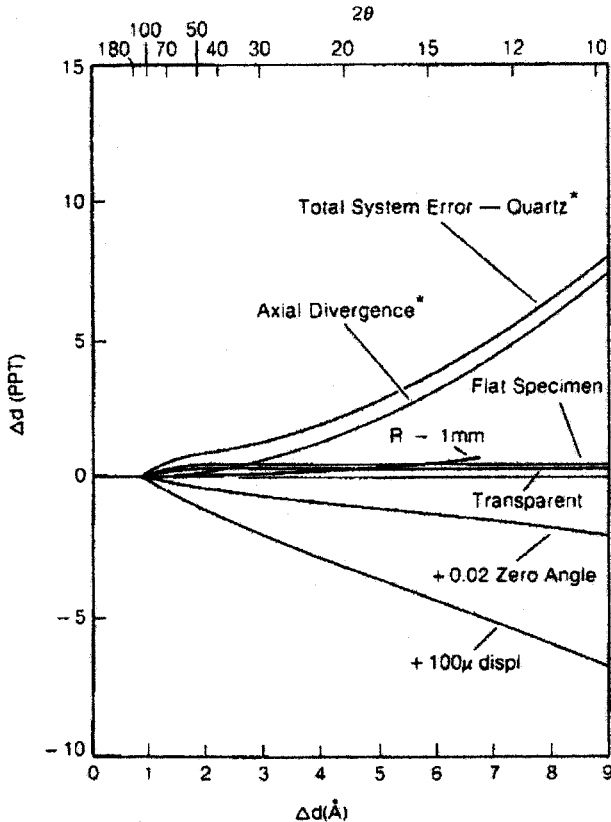


Figure 16. Plot of the frequency of occurrence of inorganic lines of $l = 100$ of the JCPDS data base showing peak around $d = 3\text{Å}$. $T = 50$ lines peak at about $d = 1.5\text{Å}$. These point to the need for best accuracy between 20–60° 2 θ to distinguish phases with their most important lines in this region.

Errors Affecting Identification

Phase identification involves matching observed diffraction lines with characteristic lines of various pure standards. The strongest and most isolated standard lines are the ones most important for matching. In Figure 16 we have plotted the frequency of occurrence of $l = 100$ lines in the inorganic portion of the JCPDS¹⁰ data base. These are seen to peak around $d = 3\text{Å}$. The peak of the frequency distribution of $T = 50$ lines is around $d = 1.5\text{Å}$. This means one needs the best accuracy from 20–60° 2 θ to distinguish phases with their most important lines in this region. In practice one finds accuracies of $\Delta d/d \approx 1/1000$ are required for good phase identification. The best patterns presently in the data base are of this quality or better. In order to compare the degradation of accuracy due to systematic error as a function of d , the systematic errors are plotted in Figures 17–19 in $\Delta d/d$ in units of parts per thousand.

Figure 17. Effect of Δd on axial divergence.



* Theoretical curve. Probably wrong below 20° .

Figures 17-18-19. Systematic errors plotted to compare degradation of accuracy as a function of d , in $\Delta d/d$ units of parts per million.

In Figure 17 we see the effect on $\Delta d/d$ of axial divergence, flat specimen, transparency (for quartz), a $+0.02^\circ$ zero angle offset, a -1mm error in specimen to receiving slit distance and a $100\mu\text{m}$ displacement error. It is seen that displacement error is by far the largest source of error. The only other possibly significant errors are axial divergence and zero angle offset. However, as we noted before, it seems unlikely that axial divergence error is correct at low angles, i.e., large d . Furthermore, zero angle error behaves almost the same as specimen displacement error in the important region of $0-60^\circ 2\theta$.

Two other errors not normally thought of in terms of their effect on phase identification by computer search/match programs are data base d -packing precision and the experimenter's d -reporting precision. These errors are seen in Figures 18 and 19, respectively. The two most commonly used search/match programs, the PDSM component of CIS¹¹ and the Johnson/Vand search/match¹², pack the d -values for storage as integer values of $1000/d$. This introduces a very substantial random error, at least by comparison to the other systematic errors. Probably the reason this source of error has not been noted as being a serious problem until now is that typical displacement errors are of the same order of magnitude. Clearly, if displacement errors are corrected for, this packing precision is inadequate.

Figure 18. Effect of data base d -packing precision on phase identification.

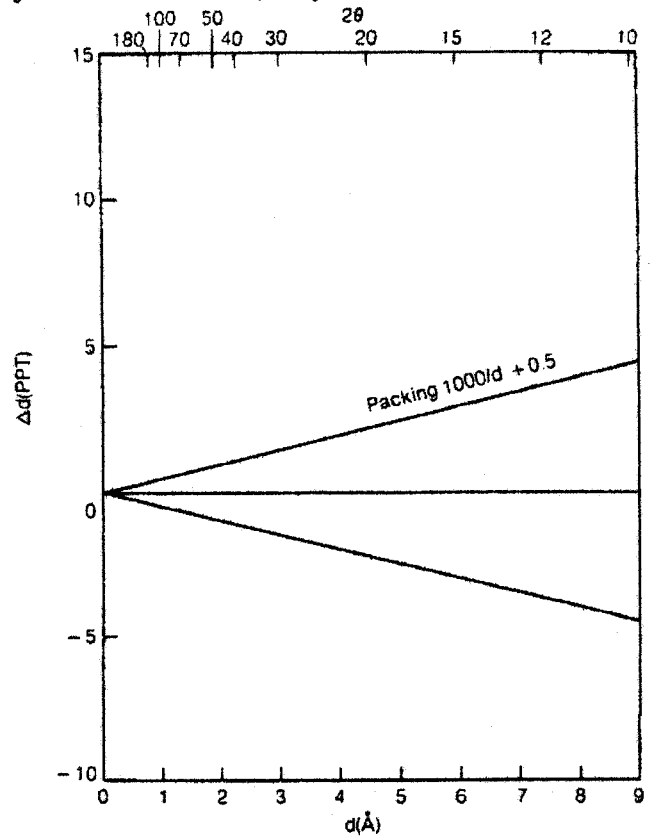
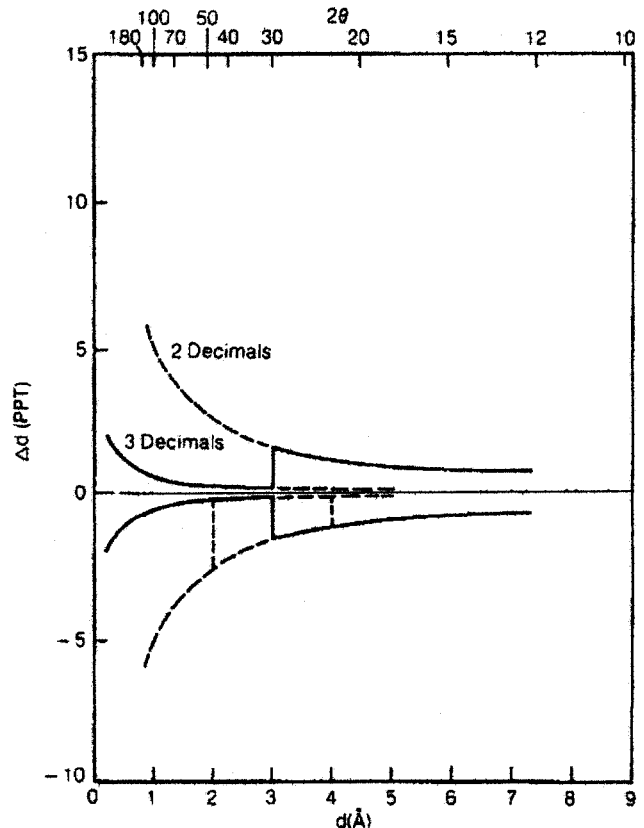


Figure 19. Effect of experimenter's d -reporting precision on phase identification.



Similarly, experimenters frequently report d-spacings to 2 places after the decimal down to about 3 Å, and thereafter to 3 decimal places. This introduces a substantial random error which has its maximum effect in the d-spacing range most crucial for phase identification. Reporting 3 decimals up to $d = 10 \text{ Å}$, even if the experimenter felt the precision not fully justified, would eliminate the introduction of this very artificial error.

This suggestion is certain to raise eyebrows of many X-ray analysts, however it is indeed well founded. When systematic errors exceed random errors, the normally accepted practice is to report all figures of accuracy out to the random error and give error bars for both random and systematic errors. As we have just seen systematic errors are larger than random errors in powder diffraction work and therefore the rule should be employed when reporting data for publication. The justification for the distinction between random and systematic errors is that while there may be a question regarding the absolute accuracy of the lines due to systematic errors, the relative accuracy (i.e., "distance" between lines) depends mainly on the random errors which are significantly smaller. Under these circumstances, if it were possible to eliminate the systematic errors in a pattern, the residual random errors should reflect measurement errors, not rounding errors.

Ordering of Errors

Based on the comparisons made in Figures 17-19 and other factors, we rated the various sources of error on a scale of 1-10, in terms of their relative importance to the problem of phase identification. We are thinking primarily in terms of inorganic rather than organic analysis. The list, seen in Table 1, is admittedly very subjective. Many experimenters might disagree with the order of certain errors, and rightly so, since it is clearly impossible to generalize across all situations encountered in phase identification. Nevertheless, it does provide a logical order in which errors can be attacked when designing a general-purpose search/match program for a computer, and that is how we have used it.

We have divided the errors into those which primarily affect d-measurements and those which primarily affect I-measurements. The right hand column indicates whether the error is essentially random or systematic in nature. Since errors add in quadrature (assuming they are independent) there is no point in trying to control a given systematic error if there is a random error which is larger. Heading the top of the list of d-errors is displacement error. Its effect is systematic, hence, if controlled, will not be the limiting error. Next, somewhat surprisingly, come the round-off errors: d-packing and d-reporting precisions. These errors are random and hence would be the limiting errors, were it not for the fact that they are artificially introduced and can therefore be reduced. The next most important random d-errors are things like broad lines, small peaks with low counting statistics, etc. Round-off errors should therefore be reduced to be less than these errors. Other systematic errors (which potentially can be controlled and/or monitored) are rated between 4-5 on our scale. Of these, we tentatively rated axial divergence highest because of some lingering doubt as to its effect on peak positions at low angles. Alignment errors like zero angle and 2:1 offsets can be monitored with external standards. Other errors like flat specimen and transparency can be corrected for theoretically.

The conclusion of this discussion is twofold:

- (1) Displacement error is the most significant systematic error and
- (2) if displacement is compensated for, the round off errors at level 6 must be reduced in order to make it worth while correcting for errors at levels 4-5.

Table 1
Relative Importance of Errors

Scale	d — Measurement Errors	I — Instrument Errors	Type
10	Displacement Error		S
9			
8			
7		Preferred Orientation	R
6	d-Packing		R
	d-Reporting		R
		Stress/Strain	R
5	Axial Divergence		S
	Zero Angle		S
		I-Reporting	R
4	Flat Specimen		S
	Transparency		S
		2:1	S
3	Spec-Rec Slit Distance		S
	Broad Lines		S
	Count Statistics	Count Statistics	R
2	Beam Uniformity		R
	α_2 Influence		
	Cocked Slits		
1	Mechanical		
0	Temp Variations		
	λ — CuK ₂		

S = Systematic Error R = Random Error

In the case of I-errors, the story is quite different. Most of the errors are random in nature, so there is no potential improvement possible in software that does not first require effort at the specimen preparation level.

Conclusions

While the intent of our exercise was to organize the various systematic and random errors affecting phase identification in order to maximize the return on time invested in designing and writing computer search/match software, there were several side benefits as well. First, it seems clear that there are a number of areas still in need of theoretical investigation. Specifically, the resolution of the unphysical divergence of the axial divergence term at low angles should be undertaken and modifications to this term as well as other errors should be developed to reflect present-day diffractometer geometries. Second, the relationship between peak and c.g. measurements should be studied. It seems likely that effective correction procedures could be developed experimentally without the necessity of developing detailed theoretical models for peak shifts. This work would be most useful for the automatic correction of systematic diffractometer errors. Third, some adjustment in the d-reporting procedures should be made to insure that no (potentially) useful information is discarded.

References Please see page 52.

Biographies

Randall H. Dow received his B.S. Degree in chemistry from the University of Idaho (1977) and is completing his M.S. in Analytical Instrumentation. These studies involve advanced chemical analysis, computer programming and electronics. He was a Teaching Assistant, Dept. of Chemistry, Oregon State University, Corvallis, Oregon, and is now a Research Assistant at OSU's School of Oceanography.

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Joseph I. Goldstein received his B.S. (1960), S.M. (1962) and Sc.D. (1964) from MIT. After holding positions in the Smithsonian Astrophysical Observatory, NASA-Goddard Space Flight Center, and the University of Maryland, he moved to Lehigh University in 1968. He is the T.L. Diamond Distinguished Professor of Metallurgy and Assistant Vice-President for Research. A past President of the Microbeam Analysis Society, he has published extensively in the field of solid state phase transformations and associated diffusion phenomena. He is the major author of a textbook, Scanning Electron Microscopy and X-ray Microanalysis, and an editor of the text, Introduction to Analytical Electron Microscopy.

W. M. A. Hax received his Ph.D. (1974) in biochemistry from the University of Utrecht. His thesis work involved a combined physical and bio-chemical study of passive cell communication. He moved to N.V. Philips' Research Laboratory in 1975, where he was involved in a project concerning storage of information in the brain. At present he is a member of the Philips Application Laboratory, Electron Optics.

Ron Jenkins is the Principal Scientist for X-Ray Analysis with Philips Electronic Instruments, Inc. He received a Licentiate degree in Chemistry from Oxford Polytechnic in England and a Doctorate in Chemical Physics from the Polytechnic Institute of New York in Brooklyn. Dr. Jenkins joined Philips in 1962 as Head of the Application Laboratory in England and four years later transferred to a similar function in the Netherlands. He moved to the U.S. in 1971. Prior to joining Philips, Dr. Jenkins worked for Esso Research in the U.K., as an Analytical Chemist. A member of the Royal Institute of Chemistry, the Institute of Physics, the Society for Applied Spectroscopy, the Mineralogical Society, the American Institute of Chemists, the Canadian Spectroscopy Society and the Crystallographic Association, Dr. Jenkins has published six books and about 100 pages in X-Ray Diffraction and Spectroscopy. He has lectured on these subjects all over the world and is Editor-in-Chief of the International Journal of X-Ray Spectrometry.

Walter N. Schreiner, Philips Laboratories, Inc., Briarcliff N.Y., is program leader for Automated Powder Diffractometer Development. He is responsible for developing mathematical and analytical diffractometry techniques and the associated hardware and software for mini- and microcomputer controlled diffractometers. Previously as a research associate at Brookhaven National Laboratories he developed pattern recognition programs for the automatic reconstruction of particle tracks in spark chambers while studying proton-proton interactions with the alternating gradient synchrotron. He received his Ph.D. in physics magna cum laude from Virginia Polytechnic Institute and State University in 1973. After receiving his M.A. from the University of California at Santa Barbara in 1965, he taught graduate physics at the Universidad Del Norte in Antofagasta, Chile, while in the Peace Corps. He is a member of Sigma Phi Sigma, Pi Mu Epsilon, American Physical Society and the Joint Committee on Powder Diffraction Standards.

Bernard Squires received his B.S. (1974) and M.S. (1977) in Physical Chemistry from Niagara University. Following that he was employed as a Senior Chemist at NL Industries, ICD Division, in Niagara Falls, N.Y., in the Quality Assurance Laboratory. Mr. Squires is presently working at Philips Electronic Instruments in the X-ray Applications Laboratory, supporting X-ray diffraction instrumentation.

Carol Surdukowski, who writes software for analytical X-ray instrumentation at Philips Laboratories, Briarcliff Manor, N.Y., has a B.S. in physics (1976) from Fairleigh Dickinson University and an M.A. in astronomy from Columbia University.

Curt Villamizar is presently a software engineer at Philips Electronic Instruments and has been intimately involved with design and coding of the APD3600. He received his B.E. in electrical engineering from Stevens Institute of Technology in 1978.

David B. Williams received his B.A., M.A. and Ph.D. in Metallurgy and Materials Science from the University of Cambridge, England. After three years postdoctoral research there he took an assistant professorship at Lehigh University where he is now associate professor and director of the Electron Optical Laboratory. His research is primarily on the application of microanalytical techniques and electron microscopy to the study of phase transformations and solute segregation phenomena in engineering materials. He has published over 50 technical articles in this area.

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3. E.R. Pike, "Counter Diffractometer — The Effect of Vertical Divergence on the Displacement and Breadth of Powder Diffraction Lines", *J. Sci. Instr.*, 34, (1957) and *ibid.* 36, 52 (1959).
4. Pike gives the axial divergence term as $\langle 2E \rangle = -\frac{1}{3} \left(\frac{H^2}{S} \right) [q, \cot \theta \{ q^2 + \csc 2\theta \}]$ where Q_1 and Q_2 are both positive definite, and H and S are geometrical lengths.
5. See for example, J. Ladell, W. Parrish, J. Taylor, *Acta Cryst.* 10, 741 (1957) and *ibid.* 12, 253 (1959).
6. In addition to references 1-3, see also several articles in *Advances in X-Ray Diffractometry and X-Ray Spectroscopy*, ed. W. Parrish, Centrex Pub. Co., Eindhoven, Netherlands (1962) and references therein.
7. "The APD-3600, A New Dimension in Qualitative and Quantitative X-Ray Powder Diffractometry", R. Jenkins, Y. Hahn, S. Peariman, W.N. Schreiner, *Norelco Reporter* 26, 1 (1979).
8. The formula is $\Delta(2\theta) = \sigma^2 \cot \theta / 343.7748$ where σ is the divergence angle in degrees. See, e.g., Wilson A.J.C., *J. Sci. Instr.* 27, 321-325 (1950).
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