

The Polarization Ratio of Crystal Monochromators

A Survey by the International Union of Crystallography Commission on Crystallographic Apparatus

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Abstract

A tabulation of some 40 measured values of the polarization ratio K (a measure of the fractional polarization introduced into an X-ray beam by a crystal monochromator) is presented. The values may be represented through the parameter n given by $K = \cos^n 2\theta_M$. The measured values of n cluster around unity and the theoretical rationale for this result is discussed. Possible explanations of outlying values are considered. A recommendation is made that the polarization ratio of an apparatus be measured using a direct method whenever possible, but methods for estimating a value of K are also given.

Introduction

Typically, the beam in a crystal-monochromated X-ray diffraction experiment is partially polarized, and the degree of polarization must be known in order to use the correct polarization factor in the interpretation of the data. Many authors tacitly assume that the degree of polarization may be adequately estimated by considering that the crystal monochromator acts as an ideally mosaic diffractor placed in an otherwise unpolarized beam of characteristic radiation. Actually, most measurements have shown that this assumption is not correct and that the deviation from its prediction is significant by modern standards of accuracy in the case of radiation of wavelength greater than about 1 Å. It is clearly of some importance to establish whether these measurements are not typical of diffraction apparatus or whether those crystallographers making use of the tacit assumption should reassess their procedures. Accordingly, the Commission on Crystallographic Apparatus of the International Union of Crystallography (International Union of Crystallography, 1978) instituted a survey of polarization ratios. The call for response to the survey offered additional material on measuring, understanding, and reporting polarization ratios. At about the same time, Le Page, Gabe & Calvert (1979) published a simple technique for measuring polarization ratios. In spite of this activity, there was very

little response to the survey, which was extended through the International Union of Crystallography 1981 Congress, at which additional invitations to respond were proffered. These did bring forth additional responses, and it is therefore now appropriate to publish all the information which has come to the attention of the survey organizer. We will give a short discussion of polarization ratios, sufficient to understand the reported values, then a table of results, and finally some brief comments on the values.

Discussion of polarization ratios

We may distinguish a beam polarization ratio K from a sample polarization ratio α . This latter may be used to characterize specimen perfection as exemplified by the work of Chandrasekhar and coworkers (*e.g.* Chandrasekhar, Ramaseshan & Singh, 1969) and by the extensive research of Olekhovich and associates (*e.g.* Olekhovich, Karpei & Markovich, 1978), unfortunately, for the present purpose, mostly on semi-conducting materials rather than on typical monochromating materials. It is convenient to distinguish two meaningful cases of sample polarization ratios. At one extreme, we have the ratio of the reflectivity of the sample for a well-collimated beam of each of the two polarizations. This parameter may be called α_s (because the angular distribution of the beam is a δ function) and is clearly a function of the angular setting of the sample. The quantity α_s may be called the reflectivity polarization ratio or polarization coefficient. If the angular setting of the sample (of monochromating material) is not specified, it may be assumed that the polarization coefficient at maximum reflecting power is being quoted. At the other extreme, we may consider the integrated polarization ratio given by $\alpha_p = \rho_{\parallel} / \rho_{\perp}$, the ratio of the two integrated intensities.

The beam polarization ratio is not a property of a material, but rather of an apparatus. For an arrangement with no polarization-dependent components after the sample, it is the ratio of the effective power (incident on the sample) in each of the two polariza-

tion states. In principle, because of non-uniformity in the beam and angularly dependent absorption effects in the sample, the beam polarization ratio might not be independent of diffractometer settings. In practice, a constant value is usually assumed. In the case that the experimental beam is prepared by diffracting a well-collimated unpolarized source beam from a monochromator with a polarization coefficient α_s , we would find that the experimental beam has a polarization ratio $K_s = \alpha_s$. If, on the other hand, the source beam had a uniformly illuminated broad angular distribution, we would have $K_p = \alpha_p$. The optimum geometry for maximum monochromated power usually is intermediate between these extremes. Thus the observed value of K , even for an unpolarized source beam, is given by some sort of an averaged sample polarization ratio α . Because the appropriate weighting function has no particular significance except with respect to an individual apparatus, this value of α does not effectively characterize the monochromator material. Usually, however, α would be expected to lie between α_s and α_p and thus knowledge of these two extremes would delimit the possible range of α and hence of K (for an unpolarized source beam).

Similar reasoning applies in the case of a diffracted-beam monochromator. The relevant value of α would involve a weighting function that depends on the angular and spatial distribution of the beam incident on the monochromator. These distributions are more likely to depend on diffractometer settings than they are in the case of an incident-beam monochromator. Nevertheless, to some approximation, we may define an effective apparatus polarization ratio, conventionally also called K . For an unpolarized incident beam, K would still be expected to lie between α_s and α_p .

Values of K can be measured by a number of different methods, which can be broadly characterized as 'direct' or 'indirect'. The direct methods are those which give the beam polarization ratio directly as the quotient of two measured quantities. Several of these methods are discussed by Suortti & Jennings (1977), but the most convenient one for 0.5–1% accuracy is that described by Le Page *et al.* (1979) and in the IUCr announcement (International Union of Crystallography, 1978, still available from L. D. Jennings). This method makes use of an amorphous sample scattering at 90° in each of two orthogonal planes. Direct methods can be cumbersome for determination of the apparatus polarization ratio in the case of a diffracted-beam monochromator; although each of the two polarizations can be selected with a Borrmann polarizer or 90° scattering, it is difficult to make the divergence conditions identical in the two measurements.

Indirect methods require more complicated analysis. For example, one can infer approximate values

of an apparatus polarization ratio from measurements of the integrated intensity of the monochromator or of the two extremes of its sample polarization ratio. However, the only indirect method used in any of the work reported here is the comparison method introduced by Miyake, Togawa & Hosoya (1964). Their technique is to compare relative integrated intensities obtained with filtered, presumably unpolarized, characteristic radiation to those obtained with a monochromated apparatus with unknown polarization ratio. This method requires accurate comparison of integrated intensities using different background subtraction techniques and also knowledge of the extinction properties of the sample. The K value is obtained by letting it be a parameter determined by a least-squares fit to the comparison. Although Vincent & Flack (1980) have recently supported the use of this technique, the difficulties in its implementation have been emphasized by Mathieson (1982) and DeMarco, Jennings, Mazzone & Sacchetti (1981).

The survey by the Commission on Crystallographic Apparatus

The IUCr survey was specifically directed toward K values. Therefore, all measured K values known to the author are entered in Table 1. In addition, the above discussion shows that α values are of substantial interest in assessing the expected range of K values. Unfortunately, most measurements of α have been on materials which are not customarily used as monochromators. A few values for the important practical case of graphite of Cu $K\alpha$ are given in Table 1. Insofar as the information is available, the table indicates whether the monochromator was before or after the sample and whether a direct or comparison method was employed. Further useful information was available in so few cases that it did not seem worth while to include it.

When polarization ratios at various wavelengths are considered, it is convenient to define a parameter n through the relation $K = \cos^n 2\theta_M$, where θ_M is the monochromator Bragg angle. We may similarly characterize a sample polarization ratio through $\alpha = \cos^m 2\theta$. The n or m values are listed in Table 1. Clearly, the constraints on values of polarization ratio could equally well be discussed in terms of the n and m values.

Various available extinction theories yield a relationship between m and the extinction coefficient y , as shown, for example, in the papers of Jennings (1968, 1981). All theories limit the range of m from zero to two; this result clearly applies to the n values of apparatus polarization ratios if the only polarizing component is a crystal monochromator. Furthermore, if the y value for the monochromator were known, the various theories suggest a comparatively limited

Table 1. *Measured values of polarization ratios*

A = monochromator after the sample (in the diffracted beam).
B = monochromator before the sample (in the incident beam).
C = comparison method. *D* = a direct method. *K* is an apparatus polarization ratio, characterized by the parameter *n*, and α is a sample polarization ratio, characterized by *m*, as detailed in the text.

Entry number	Conditions	<i>K</i> or α	<i>n</i> or <i>m</i>	Reference
Graphite @ Cr <i>K</i> α ;	<i>cos 2θ = 0.766</i>			
1	<i>A, C</i>	0.75 (4)	1.08	Altree-Williams & Jordan (1980)
Graphite @ Co <i>K</i> α ;	<i>cos 2θ = 0.857</i>			
2	<i>B, D</i>	0.919 (4)	0.54	DeMarco <i>et al.</i> (1981)
Graphite @ Cu <i>K</i> α ;	<i>cos 2θ = 0.894</i>			
3	<i>B, C</i>	0.860 (14)	1.35	Vincent & Flack (1980)
4	<i>C</i>	0.86	1.35	Hope (1971)
5	<i>D</i>	0.89	1.04	Sparks (1974)
6	<i>B, D</i>	0.896 (6)	0.98	Annaka (1981)
7	<i>B, D</i>	0.897 (5)	0.97	Le Page, Gabe & Calvert (1979)
8	<i>B, D</i>	0.905	0.89	Suortti & Jennings (1977)
9	<i>A, D</i>	0.906 (8)	0.88	Valvoda (1981)
10	<i>B, D</i>	0.908 (5)	0.86	Le Page, Gabe & Calvert (1979)
11	<i>B, D</i>	0.925	0.70	Suortti & Jennings (1977)
12	<i>A, C</i>	0.93 (4)	0.65	Altree-Williams & Jordan (1980)
13a	<i>B, D</i>	0.985	0.13	Cohen (1982)
13b	<i>B, D</i>	0.989	0.10	Bardhan & Cohen (1976)
14a	α_s	0.905 (14)	0.89	Calvert, Killean & Mathieson (1974a, b)
14b	α_s	0.888 (18)	0.99	Calvert <i>et al.</i> (1974a, b)
15	α_p	0.803	1.96	Olekhovich <i>et al.</i> (1981)
16	α_p	0.899	0.95	Olekhovich <i>et al.</i> (1981)
Graphite @ Mo <i>K</i> α ;	<i>cos 2θ = 0.978</i>			
17	<i>B, C</i>	0.907 (11)	4.29	Vincent & Flack (1980)
18	<i>B, D</i>	0.970 (3)	1.34	Le Page, Gabe & Calvert (1979)
19a	<i>B, D</i>	0.969 (3)	1.42	Le Page, Gabe & Calvert (1979)
19b	<i>B, D</i>	0.973 (5)	1.20	Le Page, Gabe & Calvert (1979)
Graphite @ Ag <i>K</i> α ;	<i>cos 2θ = 0.986</i>			
20	<i>B, C</i>	0.805 (11)	15.4	Vincent & Flack (1980)
21	<i>B, D</i>	1.000 (2)	0.0	DeMarco <i>et al.</i> (1981)
LiF @ Co <i>K</i> α ;	<i>cos 2θ = 0.605</i>			
22	<i>B, D</i>	0.60 (2)	1.02	Suortti (1983)
LiF @ Cu <i>K</i> α ;	<i>cos 2θ = 0.707</i>			
23	<i>B, D</i>	0.62 (1)	1.38	Reid (1981)
24	<i>B, C</i>	0.624	1.36	Miyake, Togawa & Hosoya (1964)
25	<i>B, D</i>	0.629	1.34	Corella & Batterman (1970)
26	<i>D</i>	0.65	1.24	Sparks (1974)
27	<i>B, D</i>	0.664 (5)	1.18	Trucano & Batterman (1968)
28	<i>D</i>	0.69	1.07	Sparks (1974)
29	<i>B, D</i>	0.707 (7)	1.00	Walker (1977)
30	<i>B, D</i>	0.722 (2)	0.94	Jennings (1968)
31	<i>B, D</i>	0.730 (6)	0.91	Annaka (1981)
32	<i>B, D</i>	0.730	0.91	Suortti & Jennings (1977)
33	<i>B, D</i>	0.780	0.72	Suortti & Jennings (1977)
LiF @ Mo <i>K</i> α ;	<i>cos 2θ = 0.938</i>			
34	<i>B, D</i>	0.93 (1)	1.13	Suortti (1983)
35	<i>D</i>	0.944 (2)	0.90	Reid (1981)
36	<i>B, D</i>	0.96	0.63	Chipman & Jennings (1977)
Quartz @ Cu <i>K</i> α ;	<i>cos 2θ = 0.894</i>			
37	<i>C</i>	0.825	1.71	Hosoya (1968)
38	<i>A, C</i>	0.90 (2)	0.94	Linkoaho, Rantavuori & Korhonen (1971)
39	<i>B, D</i>	0.905	0.89	Suortti & Jennings (1977)
40	<i>B, D</i>	0.915	0.79	Suortti & Jennings (1977)
41		0.94 (2)	0.55	Stephan & Loschau (1976)
42		0.95 (2)	0.46	Stephan & Loschau (1976)
Ge @ Cu <i>K</i> α ;	<i>cos 2θ = 0.888</i>			
43	<i>D</i>	0.94 (2)	0.52	Olekhovich (1969)

Notes

Entries 8 and 11 represent measurements on the same material: the former is more nearly *K α* , the latter more nearly *K β* .

Entry 13a is an alternative recent measurement of the apparatus of 13b, as discussed in the text.

Entry 14a was not corrected for secondary extinction and is thus comparable to the other entries; 14b is the same data corrected for secondary extinction.

Entries 15 and 16 represent the extreme cases of the 12 samples studied.

Entry 19a includes both characteristic and continuum radiation and is thus comparable to the other entries; 19b is derived from the same data with the continuum removed.

The following pairs of entries represent different specimens studied in otherwise nearly identical conditions: 7 & 10; 15 & 16; 18 & 19; 26 & 28; 32 & 33; and 39 & 40.

possible range of *m* values. Unfortunately, very few integrated intensities for monochromators have been reported, but the work of Jennings (1968, 1981) and of Lawrence (1982) suggests a typical range of γ from 0.3 to 0.4. For graphite in symmetrical reflection at Cu *K* α , the theories considered by Jennings (1981, Figs. 2 and 3) give corresponding *m* values from 0.8 to 1.2. This result is not much changed for other typical monochromators at crystallographic wavelengths (Jennings, 1968, and unpublished results).

The *n* and *m* values of Table 1, for the most part, lie near this expected range, 0.8 to 1.2, supporting the theoretical reasoning. We will therefore make some general remarks using the language of these theories and then consider specifically some of the entries in Table 1 which illustrate significant points.

In many geometries, it is desirable to arrange the monochromator for maximum reflecting power. In general, such an arrangement leads to a lower extinction coefficient γ and to *n* values near to or less than unity. (This does *not* imply that the monochromator is a nearly perfect crystal; this result holds true because of sizeable secondary extinction.) Some monochromators may not be adjusted for high reflectivity, and in these cases *n* values near 2 are plausible. In any case, a few workers studied monochromator materials with varying rocking-curve widths; the trend toward smaller *n* values with narrowing rocking curves (higher reflecting power, smaller extinction coefficient) is unmistakable, though there is a great variation from sample to sample (Suortti & Jennings, 1977; Le Page *et al.*, 1979; and, especially, Olekhovich, Markovich, Olekhovich & Poluchankina, 1981).

The only other trend observed is that the comparison method gave, on average, higher *n* values than the direct methods. No information is available on whether the apparatus studied with the comparison method, on average, used less-efficient monochromators, or whether there is a shortcoming in one of the methods.

It is of interest to examine, in Table 1, each of the entries which is outside the plausible range of *n* values. Entry 21 illustrates the important point that a small amount of continuum is generally included as part of the 'monochromatic' beam. To estimate the effect of this included continuum on the polarization ratio, consider the geometry applicable to entry 21: the exciting electron beam is in the plane of diffraction of the monochromator. The beam incident on the monochromator contains four components: two continuum components polarized in and perpendicular to the plane of diffraction so that their intensity ratio is $C_{\parallel}/C_{\perp} = (1 + P)/(1 - P)$; and two unpolarized components arising from the characteristic line, $L_{\parallel} = L_{\perp}$. Here *P* is the fractional polarization of the continuum and is positive for the geometry and sign convention chosen. The monochromator reflects each of these

components with a reflectivity ratio $R_{\parallel}/R_{\perp} = \cos^m 2\theta_M$. If then the fraction of the beam power arising from the continuum is f , it is easy to show that

$$K = \cos^m 2\theta_M \frac{1+fP}{1-fP}.$$

Accurate values of m , f and P are not readily available, but rough estimates may be made. Typical values of P might be 20–30% as discussed, for example, by Compton & Allison (1935). Values of f , typically about 1–3%, may be obtained from a dispersive scan of the beam or from the power ratio when the monochromator is set to reflect the continuum rather than the characteristic radiation. Typical m values for hard radiation are somewhat lower than the Cu $K\alpha$ values discussed above (Jennings, 1968) and so might be in the range 0.5 to 1.0. Thus the result of entry 21 can be explained by values in these typical ranges, such as $m = 0.5$, $P = 0.2$ and $f = 0.018$ or $m = 1.0$, $P = 0.3$ and $f = 0.023$.

From this discussion, it can be seen that the measurement of the beam polarization ratio does not accurately determine the m value characterizing the sample polarization ratio in this case. This situation comes about because of the small possible range of polarization ratios and from the presumably greater continuum contamination for hard radiation. For softer radiations, the n values of Table 1 probably characterize the sample polarization ratios reasonably well. Furthermore, by using special techniques, the continuum can be subtracted as part of the background (entry 19*b*), but such procedures are not usually employed. In fact, most authors do not state the orientation of the exciting electron beam, so it is not possible to establish whether the continuum contribution increases or decreases their K value.

The measurement for entry 13*b* was carried out using a different radiation from that used in the concomitant experiment. A later measurement, entry 13*a*, giving substantially the same result, was carefully carried out without disturbing the experimental arrangement. The apparatus uses quite large divergences, and it may be that a relatively large amount of continuum was included, making the above discussion of small n values applicable.

The measurements of entries 17 and 20 are stated to be of high accuracy and were the primary objective of the authors' experimental program. Unfortunately they do not state the geometrical parameters, do not report having verified the unusual results with a direct method, and do not give a rationale for the results. It may be relevant that the experiments were carried out with a sample displaying higher extinction than in other implementations of the comparison method. It remains to be established with certainty whether there is some considerable difficulty in the application of the comparison method, as suggested by Mathieson

(1982), or whether some physical principles, unclear to this author, must be considered.

Conclusions and recommendations

In summary, the author offers these recommendations based on the results shown in Table 1 and on other experience..

1. For accurate work, especially for radiations of wavelength greater than 1 Å, the polarization ratio of a typical crystal-monochromated apparatus must be established.

2. If at all possible, measure the apparatus polarization ratio K using a direct method.

3. If such a measurement is not feasible, a reasonable first guess is that $K = \cos^n 2\theta_M$, with $n = 1$. This is *not* tantamount to an assumption that the monochromating crystal is nearly ideally perfect.

4. If the set-up is of relatively high efficiency, lower the n value somewhat; this situation is valid for a relatively narrow crystal rocking curve and/or good collimation conditions (as typically apply to a bent monochromator). Conversely, raise the n value somewhat for a low-efficiency set-up.

5. Establish from the geometry whether the continuum contribution increases or decreases K . (The polarization is along the exciting electron beam.) The meager information available suggests that a typical magnitude for this change in K is about 0.01 (assuming, of course, that the predominant component of the beam is initially unpolarized characteristic radiation).

6. Procedures for dealing with polarization ratios are not well established. Therefore, a publication listing a polarization ratio should detail relevant geometrical aspects and the methods used for determining the ratio, as well as its value.

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Treatment of Secondary Extinction and Multiple Scattering in Polarized Neutron Scattering: An Improved Method.

I. Method

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Abstract

A new method for the treatment of secondary extinction in polarized neutron diffraction data has been developed. As in previous models, the Zachariasen solutions to the Darwin intensity transfer equations are used, but in this case the extinction corrections are made on a point-by-point basis across the rocking curve and the corrections are determined by the absolute reflectivity at each point. There are no adjustable parameters (other than background). Measure-

ment of the reflectivity also provides a simple test for multiple scattering, since the sum of diffracted and transmitted intensities should equal the direct-beam intensity, corrected for absorption, if no multiple scattering is present. The present method should give more reliable results than parametrized models where the correlation between the extinction and other parameters, such as the scale factor and temperature factors, are important.

1. Introduction

Scattering of polarized neutrons has provided nearly all of the information presently available about the

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