

of the other signs. Maximization of (IV-7) over all the possible values of $(s_1 \dots s_p)$, assuming \vec{K} to have a fixed value, will give the most probable set of these signs. (IV-7) gives rise to expression (23); in fact, since B_1 does not depend on any sign, it clearly follows that:

$$\text{Max } P(s_1 \dots s_p) = \text{Max } B_2(s_1 \dots s_p). \quad (\text{IV-8})$$

Remembering the last equation in (IV-5), we may easily see that (23) and (IV-8) are equivalent.

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Intrinsic and Systematic Multiple Diffraction

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The geometric conditions under which intrinsic multiple diffraction can occur have been examined for the single-crystal orienter technique in the equatorial plane, and for the precession camera technique. The conditions for the single-crystal orienter are the same that have already been found for normal beam and equi-inclination techniques by Zachariasen, and in part by Fankuchen and co-workers. If a crystal is oriented with a symmetry axis parallel to, or a symmetry plane normal to, the rotation axis (φ axis) then intrinsic multiple diffraction will occur. The consequences of the conditions are different, however. For the normal beam and equi-inclination cases reflections on nonzero layer lines will be recorded under conditions of double and triple diffraction, respectively, and the situation is both intrinsic and systematic. For the single-crystal orienter the situation is intrinsic but not always systematic. Depending both on the crystal symmetry and the indices of the reflections the multiplicities may be triple, quintuple, septuple, 11-fold, or 15-fold. For the precession camera the situation is not intrinsic. However, if a crystal is again oriented with a symmetry axis parallel to, or a symmetry plane normal to, the rotation axis (in this case the spindle axis) a systematic case can be created. If the precession angle $\bar{\mu}$ is set at $\bar{\mu} = \cos^{-1}(d^*/2)$, where d^* is the reciprocal lattice spacing from the zero level to an upper level, then all reflections on the zero level are recorded under conditions of triple diffraction. The possibilities for nonsystematic cases with the precession camera are more interesting. The conditions for multiple diffraction of selected groups of zero level reflections can be created or avoided at will by the choice of $\bar{\mu}$, regardless of crystal symmetry or crystal orientation. In principle this should permit direct observation of the effects of multiple diffraction on intensities.

Zachariasen (1965) has recently emphasized that most intensity measurements reported in the literature, and used for structure determination, have been made under conditions of multiple diffraction. For normal beam techniques (rotating crystal, oscillating crystal, or Weissenberg) all reflections on nonzero layer lines are obtained under conditions of double diffraction if a crystal is oriented with a symmetry axis parallel to, or a symmetry plane normal to, the rotation axis*. For the

equi-inclination Weissenberg technique all reflections on nonzero layer lines are obtained under conditions of triple diffraction if a crystal is oriented as above.† Zachariasen also illustrated two special cases where certain zero layer line reflections are subject to triple or quintuple diffraction when a fourfold or sixfold symmetry axis is normal to the rotation axis. In addition Zachariasen solved the intensity equations for double, triple, and quintuple diffraction for a plane,

* Depending on the Bravais lattice there are two possibilities: Either all reflections on every nonzero layer line, or all reflections on every third layer line, will be subject to double diffraction.

† Depending on the Bravais lattice there are three possibilities: All reflections either on every nonzero layer line, or on every second layer line, or on every third layer line, will be subject to triple diffraction.

parallel plate crystal with a secondary extinction coefficient of 200 and obtained numerical values of the multiple diffraction corrections. The results indicate that strong reflections are weakened, and weak reflections are strengthened by multiple diffraction, the magnitude of the effects increasing with increase in multiplicity of diffraction. Systematic multiple diffraction in the equi-inclination case was recognized earlier by Fankuchen (Fankuchen & Williamson, 1956; Yakel & Fankuchen, 1962). However, the full significance of the effect and its widespread occurrence in almost every technique did not become clear to me until the appearance of Zachariasen's work. It is the purpose of the present paper to indicate the conditions under which multiple diffraction occurs for the single-crystal orienter technique, where all measurements are made in the equatorial plane, and for the precession camera technique.

In the discussion that follows the terms *intrinsic* and *systematic* will be applied to multiple diffraction. If, with a given crystal symmetry and orientation, and a given diffraction technique, it is impossible to avoid conditions of multiple diffraction for at least a portion of the reflections, these reflections and the technique will be said to be subject to intrinsic multiple diffraction. If an entire class of reflections (for example all the reflections on a given layer line) is recorded under conditions of multiple diffraction, and the multiplicity of diffraction is uniform throughout the class, then the reflections and the technique will be said to be subject to systematic multiple diffraction. These definitions are introduced because systematic multiple diffraction may not be intrinsic, and intrinsic multiple diffraction may not be systematic. For the normal beam and equi-inclination cases, the multiple diffraction is both intrinsic and systematic. For the single-crystal orienter the case will prove to be intrinsic but not always systematic. For the precession camera there is one case which is systematic but not intrinsic, and an entire class of cases which are neither systematic nor intrinsic.

Single-crystal orienter technique

Consider a diffractometer and single-crystal orienter which are arranged with the source and detector in the horizontal plane. When the crystal and detector are adjusted to record a reflection a reciprocal lattice point lies somewhere on the horizontal equator of the sphere. Let a vertical plane pass through the lattice point and the origin of the reciprocal lattice. The intersection of the vertical plane and the sphere defines a vertical circle of reflection. If the crystal is so oriented that a vertical reciprocal lattice plane coincides with the vertical circle of reflection then the possibility of intrinsic multiple diffraction exists.

The conditions for intrinsic multiple diffraction with the single-crystal orienter can be found by considering three questions:

1. Is there a reciprocal lattice plane coincident with the vertical circle of reflection?
2. If so what is the symmetry of the reciprocal lattice plane?
3. What systematic effects are caused by the reciprocal lattice plane symmetry?

The answer to the first question is straightforward. If the crystal is oriented with a reciprocal lattice vector along the rotation axis (the φ axis of the single-crystal orienter) there will be a reciprocal lattice plane coincident with the vertical circle of reflection.

Six alternatives occur for the second question. There are five types of reciprocal lattice plane which correspond to true plane lattices: oblique, rectangular, centered rectangular, hexagonal, and square. For our purposes it is necessary to add a sixth type which will be called rhombohedral rectangular. Plane lattices of this triply primitive rectangular type will be encountered when a cubic crystal is oriented with a cube diagonal along the rotation axis, or when a rhombohedral crystal is oriented with its trigonal axis along the rotation axis.

In discussing the third question an unconventional nomenclature will be used. All points in a reciprocal lattice plane will be defined in terms of a pair of reciprocal lattice plane vectors, \bar{v}_1 , \bar{v}_2 . The reflections will be identified in terms of indices p_1 , p_2 such that the vector $p_1\bar{v}_1 + p_2\bar{v}_2$ extends from the origin of the reciprocal lattice plane to the reflection p_1 , p_2 . In general the reciprocal lattice plane vectors \bar{v}_1 , \bar{v}_2 will represent compound translations in the three-dimensional reciprocal lattice, such as [224] or [220]. The reciprocal lattice plane definitions in terms of \bar{v}_1 , \bar{v}_2 are:

1. Oblique: $|\bar{v}_1| \neq |\bar{v}_2|$, $\bar{v}_1 \cdot \bar{v}_2 \neq 0$
2. Rectangular: $|\bar{v}_1| \neq |\bar{v}_2|$, $\bar{v}_1 \cdot \bar{v}_2 = 0$
3. Centered rectangular: as for rectangular plus an additional lattice point at $\frac{1}{2}(\bar{v}_1 + \bar{v}_2)$ from any given lattice point. Half the reflections have p_1 , p_2 integral, half have p_1 , p_2 nonintegral.
4. Rhombohedral rectangular: as for rectangular plus two additional lattice points at $\frac{1}{3}(\bar{v}_1 + \bar{v}_2)$, $\frac{2}{3}(\bar{v}_1 + \bar{v}_2)$ or at $-\frac{1}{3}(\bar{v}_1 + \bar{v}_2)$, $-\frac{2}{3}(\bar{v}_1 + \bar{v}_2)$ from any given lattice point. One-third of the reflections have p_1 , p_2 integral, two-thirds have p_1 , p_2 nonintegral.
5. Hexagonal: $|\bar{v}_1| = |\bar{v}_2|$, $\bar{v}_1 \cdot \bar{v}_2 = (\sqrt{3}/2) |\bar{v}_1| |\bar{v}_2|$
6. Square: $|\bar{v}_1| = |\bar{v}_2|$, $\bar{v}_1 \cdot \bar{v}_2 = 0$

A convenient graphical construction for studying multiple diffraction on reciprocal lattice planes is indicated in Fig. 1. The conditions for reflection of 1,2 (or 2,1) and the second, third and fourth order on a square lattice are illustrated. The straight line represents a projection of the equatorial plane of the sphere which is normal to the figure. Four circles of reflection are shown which will occur in succession when the spectrometer is adjusted to record the 1,2; 2,4; 3,6; and 4,8 reflections. It is apparent that for the 1,2 reflection the first and third orders will be subject to triple diffraction, while the second and fourth orders will be subject to septuple diffraction. This simple type

of construction can be used for any reflection on any type of reciprocal lattice plane. For all the reciprocal lattice planes except the square lattice the results can be generalized into a set of rules or conditions as summarized in Table 1. For the square lattice a great variety of effects are possible which have not been reduced to a set of rules. In Table 2 the effects on a square lattice are summarized for all reflections up to the type $n \cdot 7$, $n \cdot 6$. In this table n stands for the order of the reflection. Thus for the first order of 2,1 which is illustrated in Fig. 1 there is triple diffraction with 2,0 and

0,1. For the second order there is septuple diffraction with 4,0; 0,2; 3, $\bar{1}$; 1, $\bar{1}$; 1,3; and 3,3. For the third order there is triple diffraction with 6,0 and 0,3. It would appear that the effects can be summarized for the odd and even orders. However, this has not been proved and the orders which were actually investigated are indicated in a footnote to Table 2. The same statement can be made for the single-crystal orienter that has already been found for normal beam and equi-inclination techniques. If a crystal is oriented with a symmetry axis parallel to, or a symmetry plane normal to, the rotation axis (φ axis) then intrinsic multiple extinction will occur.

Table 1. *Intrinsic multiple diffraction effects encountered with the single-crystal orienter*

Type of reciprocal lattice plane	Intrinsic effects in terms of reciprocal lattice plane indices p_1, p_2
Oblique	Single diffraction for all reflections
Rectangular	<ul style="list-style-type: none"> Triple diffraction for reflections with $p_1, p_2 \neq 0$ Single diffraction for reflections with p_1 or $p_2 = 0$
Centered rectangular and rhombohedral rectangular	<ul style="list-style-type: none"> Triple diffraction for reflections with p_1, p_2 integral and $\neq 0$ Single diffraction for reflections with p_1, p_2 integral and p_1 or $p_2 = 0$ Single diffraction for reflections with p_1, p_2 nonintegral
Hexagonal	<ul style="list-style-type: none"> Quintuple diffraction for even orders with p_1 or $p_2 = 0$, or $p_1 = p_2$ 11-fold diffraction for even orders with $p_1, p_2 \neq 0$ and $p_1 \neq p_2$ Single diffraction for odd orders with p_1 or $p_2 = 0$, or $p_1 = p_2$ Triple diffraction for odd orders with $p_1, p_2 \neq 0$ and $p_1 \neq p_2$
Square	<ul style="list-style-type: none"> Triple, septuple, 11-fold, and 15-fold diffraction have been noted for even orders Single, triple, quintuple, septuple, and 11-fold diffraction have been noted for odd order

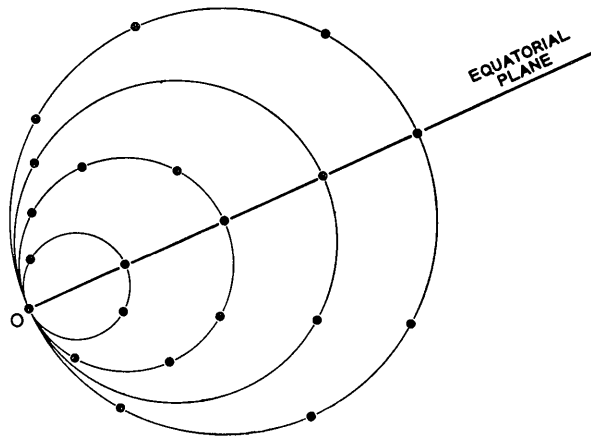


Fig. 1. Graphical construction for multiple diffraction on plane lattices. The 1,2 reflection on a square lattice and the second, third, and fourth orders are illustrated.

Zero level precession camera technique

Each of the ordinary photographic techniques has a strong analogy to a spectrometer technique. The normal beam photographic methods (rotation, oscillation, or Weissenberg) have their analogy in the normal beam spectrometer technique and the conditions for systematic multiple extinction are identical. The same is true for the equi-inclination Weissenberg method in both the photographic and spectrometer techniques. There is a limited analogy between zero level precession photography and spectrometry with the single-crystal orienter. The exploration of reciprocal space will be carried out in an equivalent manner if a crystal is mounted with a given reciprocal lattice vector along the spindle axis on the precession camera, and along the φ axis on the single-crystal orienter, and if the photographic exploration is restricted to zero level photographs. However, there are fundamental differences with respect to intrinsic multiple diffraction. To record a reflection with the spectrometer a circle of reflection must be adjusted so that a diameter of the circle is coincident with a reciprocal lattice point. As indicated in the previous section multiple diffraction is inevitable for symmetrical situations. In the precession method a circle of reflection and the lattice level to be recorded are always coincident. The precession mechanism causes the circle of reflections to traverse a circular orbit in the plane of the lattice level. On a zero level the center of the orbit is at the origin and the radius of the orbit is equal to the radius of the circle of reflection. All points on the zero level which lie inside a limiting circle whose radius is equal to the diameter of the circle of reflection will come into reflecting position twice during one traverse of the circular orbit. The radius of the circle of diffraction can be chosen at will. Therefore one can always avoid multiple diffraction, regardless of the plane lattice symmetry. Conversely, one can always deliberately cause any given reflection to undergo some type of multiple diffraction regardless of the plane lattice symmetry.

If the reciprocal lattice vectors are expressed in dimensionless units such that the radius of the sphere of reflection is unity then the radius of the circle of reflection is given by $\sin \bar{\mu}$, where $\bar{\mu}$ is the precession angle.

Table 2. *Intrinsic multiple diffraction effects encountered on square reciprocal lattice planes with the single-crystal orienter**

Reflections	Odd orders	Additional reflections	Even orders	Additional reflections
$n \cdot 1, n \cdot 0$	Single diffraction		Triple diffraction	$n \cdot 1/2, n \cdot 1/2$ $n \cdot 1/2, n \cdot \bar{1}/2$
$n \cdot 1, n \cdot 1$	Triple diffraction	$n \cdot 1, n \cdot 0$ $n \cdot 0, n \cdot 1$	Triple diffraction	
$n \cdot 2, n \cdot 1$	Triple diffraction	$n \cdot 2, n \cdot 0$ $n \cdot 0, n \cdot 1$	Septuple diffraction	$n \cdot 3/2, n \cdot \bar{1}/2$ $n \cdot 1/2, n \cdot \bar{1}/2$ $n \cdot 1/2, n \cdot 3/2$ $n \cdot 3/2, n \cdot 3/2$
$n \cdot 3, n \cdot 1$	Septuple diffraction	$n \cdot 3, n \cdot 0$ $n \cdot 2, n \cdot \bar{1}$ $n \cdot 1, n \cdot \bar{1}$ $n \cdot 0, n \cdot 1$ $n \cdot 1, n \cdot 2$ $n \cdot 2, n \cdot 2$	Septuple diffraction	
$n \cdot 3, n \cdot 2$	Triple diffraction	$n \cdot 3, n \cdot 0$ $n \cdot 0, n \cdot 2$	Septuple diffraction	$n \cdot 5/2, n \cdot \bar{1}/2$ $n \cdot 1/2, n \cdot \bar{1}/2$ $n \cdot 1/2, n \cdot 5/2$ $n \cdot 5/2, n \cdot 5/2$
$n \cdot 4, n \cdot 1$	Triple diffraction	$n \cdot 4, n \cdot 1$ $n \cdot 0, n \cdot 1$	Septuple diffraction	$n \cdot 5/2, n \cdot \bar{3}/2$ $n \cdot 3/2, n \cdot \bar{3}/2$ $n \cdot 3/2, n \cdot 5/2$ $n \cdot 5/2, n \cdot 5/2$
$n \cdot 4, n \cdot 3$	Quintuple diffraction	$n \cdot 4, n \cdot 0$ $n \cdot 2, n \cdot \bar{1}$ $n \cdot 0, n \cdot 3$ $n \cdot 2, n \cdot 4$	Septuple diffraction	$n \cdot 9/2, n \cdot 3/2$ $n \cdot \bar{1}/2, n \cdot 3/2$
$n \cdot 5, n \cdot 1$	Septuple diffraction	$n \cdot 5, n \cdot 0$ $n \cdot 3, n \cdot \bar{2}$ $n \cdot 2, n \cdot \bar{2}$ $n \cdot 0, n \cdot 1$ $n \cdot 2, n \cdot 3$ $n \cdot 3, n \cdot 3$	Septuple diffraction	
$n \cdot 5, n \cdot 2$	Triple diffraction	$n \cdot 5, n \cdot 0$ $n \cdot 0, n \cdot 2$	Septuple diffraction	$n \cdot 7/2, n \cdot \bar{3}/2$ $n \cdot 3/2, n \cdot \bar{3}/2$ $n \cdot 3/2, n \cdot 7/2$ $n \cdot 7/2, n \cdot 7/2$
$n \cdot 5, n \cdot 3$	Septuple diffraction	$n \cdot 5, n \cdot 0$ $n \cdot 4, n \cdot \bar{1}$ $n \cdot 1, n \cdot \bar{1}$ $n \cdot 0, n \cdot 3$ $n \cdot 1, n \cdot 4$ $n \cdot 4, n \cdot 4$	Septuple diffraction	
$n \cdot 5, n \cdot 4$	Triple diffraction	$n \cdot 5, n \cdot 0$ $n \cdot 0, n \cdot 4$	Septuple diffraction	$n \cdot 9/2, n \cdot \bar{1}/2$ $n \cdot 1/2, n \cdot \bar{1}/2$ $n \cdot 1/2, n \cdot 9/2$ $n \cdot 9/2, n \cdot 9/2$
$n \cdot 6, n \cdot 1$	Triple diffraction	$n \cdot 6, n \cdot 0$ $n \cdot 0, n \cdot 1$	Septuple diffraction	$n \cdot 7/2, n \cdot \bar{3}/2$ $n \cdot 5/2, n \cdot \bar{3}/2$ $n \cdot 5/2, n \cdot 7/2$ $n \cdot 7/2, n \cdot 7/2$
$n \cdot 6, n \cdot 5$	Triple diffraction	$n \cdot 6, n \cdot 0$ $n \cdot 0, n \cdot 5$	Septuple diffraction	$n \cdot 11/2, n \cdot \bar{1}/2$ $n \cdot 1/2, n \cdot \bar{1}/2$ $n \cdot 1/2, n \cdot 11/2$ $n \cdot 11/2, n \cdot 11/2$

Table 2 (cont.)

Reflections	Odd orders	Additional reflections	Even orders	Additional reflections
$n \cdot 7, n \cdot 1$	11-fold diffraction	$n \cdot 7, n \cdot 0$ $n \cdot 6, n \cdot 2$ $n \cdot 4, n \cdot 3$ $n \cdot 3, n \cdot 3$ $n \cdot 1, n \cdot 1$ $n \cdot 0, n \cdot 1$ $n \cdot 1, n \cdot 3$ $n \cdot 3, n \cdot 4$ $n \cdot 4, n \cdot 4$ $n \cdot 6, n \cdot 3$	11-fold diffraction	
$n \cdot 7, n \cdot 2$	Triple diffraction	$n \cdot 7, n \cdot 0$ $n \cdot 0, n \cdot 2$	Septuple diffraction	$n \cdot 9/2, n \cdot 3/2$ $n \cdot 5/2, n \cdot 5/2$ $n \cdot 5/2, n \cdot 9/2$ $n \cdot 9/2, n \cdot 9/2$
$n \cdot 7, n \cdot 3$	Septuple diffraction	$n \cdot 7, n \cdot 0$ $n \cdot 5, n \cdot 2$ $n \cdot 2, n \cdot 2$ $n \cdot 0, n \cdot 3$ $n \cdot 2, n \cdot 5$ $n \cdot 5, n \cdot 5$	Septuple diffraction	
$n \cdot 7, n \cdot 4$	Triple diffraction	$n \cdot 7, n \cdot 0$ $n \cdot 0, n \cdot 4$	11-fold diffraction	$n \cdot 15/2, n \cdot 5/2$ $n \cdot 15/2, n \cdot 3/2$ $n \cdot 11/2, n \cdot 3/2$ $n \cdot 3/2, n \cdot 3/2$ $n \cdot 1/2, n \cdot 3/2$ $n \cdot 1/2, n \cdot 5/2$ $n \cdot 3/2, n \cdot 11/2$ $n \cdot 11/2, n \cdot 11/2$
$n \cdot 7, n \cdot 5$	Septuple diffraction	$n \cdot 7, n \cdot 0$ $n \cdot 6, n \cdot 1$ $n \cdot 1, n \cdot 1$ $n \cdot 0, n \cdot 5$ $n \cdot 1, n \cdot 6$ $n \cdot 6, n \cdot 6$	Septuple diffraction	
$n \cdot 7, n \cdot 6$	Septuple diffraction	$n \cdot 8, n \cdot 4$ $n \cdot 8, n \cdot 2$ $n \cdot 7, n \cdot 0$ $n \cdot 1, n \cdot 2$ $n \cdot 1, n \cdot 4$ $n \cdot 0, n \cdot 6$	15-fold diffraction	$n \cdot 13/2, n \cdot 1/2$ $n \cdot 9/2, n \cdot 3/2$ $n \cdot 5/2, n \cdot 3/2$ $n \cdot 1/2, n \cdot 1/2$ $n \cdot 1/2, n \cdot 13/2$ $n \cdot 5/2, n \cdot 15/2$ $n \cdot 9/2, n \cdot 15/2$ $n \cdot 13/2, n \cdot 13/2$

* The number of orders actually investigated by graphical means for the various reflections was the following:

6 orders	4 orders	3 orders	2 orders
$n \cdot 1, n \cdot 0$	$n \cdot 2, n \cdot 1$	$n \cdot 3, n \cdot 1$;	All other reflections
$n \cdot 1, n \cdot 1$		$n \cdot 3, n \cdot 2$;	
		$n \cdot 4, n \cdot 1$;	
		$n \cdot 4, n \cdot 3$	

With an oblique plane lattice any reflection can be caused to undergo double diffraction. This is because one can always fit a circle to three noncollinear points. Consider a lattice point given by the vector $p_1\bar{v}_1$, and a second point given by the vector $p_2\bar{v}_2$, the angle between them being given by $\beta < 90^\circ$. If the precession angle is set at

$$\bar{\mu} = \sin^{-1}[(|p_1\bar{v}_1|^2 + |p_2\bar{v}_2|^2 - 2|p_1\bar{v}_1||p_2\bar{v}_2|\cos\beta)^{1/2} / 2 \sin\beta]$$

double diffraction will occur at six positions along the orbit of the circle of reflection. Six lattice points will undergo double diffraction during both passages of the circle of reflection: $p_1, 0; 0, p_2; \bar{p}_1, p_2; \bar{p}_1, 0; 0, \bar{p}_2$; and p_1, \bar{p}_2 . If $\beta = 90^\circ$ then

$$\bar{\mu} = \sin^{-1}[(|p_1\bar{v}_1|^2 + |p_2\bar{v}_2|^2)^{1/2} / 2]$$

and triple diffraction will occur at four positions along the orbit of the circle of reflection. Eight lattice points

will undergo triple diffraction during one traverse of the orbit. Four lattice points will experience two passages of the circle of reflection: $p_1, 0; 0p_2; \bar{p}_1, 0;$ and $0, \bar{p}_2$. Four lattice points will lie on the limiting circle and experience a single tangential passage of the circle of reflection: $p_1, p_2; \bar{p}_1, p_2; \bar{p}_1, \bar{p}_2;$ and p_1, \bar{p}_2 .

The possibilities for multiple diffraction are greatly increased on hexagonal or square plane lattices. A spectacular possibility on a square lattice will be given as an example. Let

$$\sin \bar{\mu} = \frac{1}{2} \sqrt{(14\bar{v}_1)^2 + (12\bar{v}_2)^2} = \sqrt{85} |\bar{v}|.$$

(This will be recognized from Table 2 as the radius of the circle of reflection that would be required on the single-crystal orienter to record the second order of the $n=7, n=6$ reflection). Fifteenfold diffraction will occur at 16 positions along the orbit of the circle of reflection. One hundred twenty-eight lattice points will undergo fifteenfold diffraction during one traverse of the orbit. One hundred twelve points will experience two passages of the circle of reflection. Sixteen points will lie on the limiting circle and experience a single tangential passage of the circle of reflection. This result is readily verified with compasses and square coordinate paper.

Unless absorption is negligible the precession camera is not well suited for upper level intensity measurements because of the complexities of the Lorentz-polarization absorption factor (Burbank & Knox, 1962). However, it is of interest to know the conditions under which upper level reflections enter into multiple diffraction with zero level reflections. On the zero level multiple diffraction is created by selecting a value of $\bar{\mu}$ which causes the circle of reflection to pass through two or more points on the plane lattice. Although very high multiplicities of diffraction can be caused for selected groups of points the process is not systematic in the sense of causing every point on a zero level to undergo multiple diffraction. When an upper level and a zero level are considered together the situation changes. The precession angle can be selected to cause a systematic condition in which every point on both levels reflects under conditions of multiple diffraction. If the crystal is oriented with a symmetry axis parallel to, or a symmetry plane normal to, the spindle axis then there will be a reciprocal lattice vector which is normal to the levels. If the magnitude of this vector is d^* , and if $\bar{\mu}$ is set to satisfy the condition $2 \cos \bar{\mu} = d^*$, then the situation indicated in Fig. 2 will occur. The zero level and the upper level are symmetrically disposed in the front and back reflection regions. The semiapex angle of the diffraction cone for the zero level is $\bar{v} = \bar{\mu}$ and the semiapex angle for the upper level is $180^\circ - \bar{v}$. The radii of the circles of reflection for each level are equal. The precession mechanism causes the upper level circle of reflection to traverse a circular orbit centered at U , while the zero level circle is traversing the orbit centered at O . The point U is always in

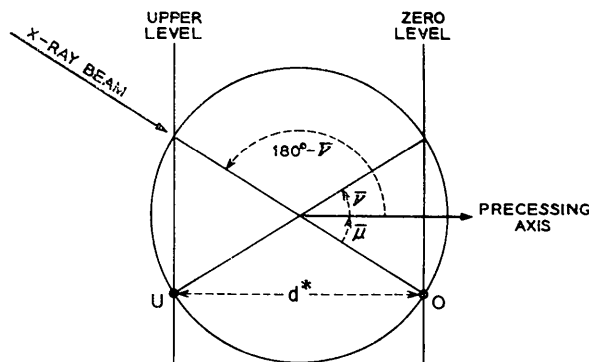


Fig. 2. Condition for systematic triple diffraction with the precession camera technique.

reflecting position and reflects the X-ray beam at $2\theta = 180^\circ - 2\bar{\mu}$. Whenever the zero level point situated at $p_1\bar{v}_1 + p_2\bar{v}_2$ from O comes into reflecting position the upper level point situated at $p_1\bar{v}_1 + p_2\bar{v}_2$ from U also comes into reflecting position and reflects the beam at $2\theta = 180^\circ$. Therefore every point on the zero level will reflect under conditions of triple diffraction. For the precession technique this upper level is unique in that it is the only one that would be free of a 'blind' spot at the center of the level if it could be photographed. There is a certain parallel between this situation and the equi-inclination Weissenberg case. There is also an important difference since for the precession technique the condition can always be avoided by setting $2 \cos \bar{\mu} \neq d^*$.

An application of the precession technique

The zero level precession technique appears to be the only method in common usage where multiple diffraction can be deliberately and conveniently introduced or avoided at will, *regardless of crystal symmetry or crystal orientation*. This offers an interesting possibility for direct experimental observation of the magnitude of multiple diffraction effects. A set of three photographs would provide the necessary observations. First the precession angle $\bar{\mu}$ would be chosen to create multiple diffraction for certain reflections. Then two additional settings would be used at $\bar{\mu} + \Delta$ and $\bar{\mu} - \Delta$, where Δ is a small increment that destroys the multiple diffraction condition for the selected reflections. The average of the intensities observed at $\bar{\mu} + \Delta$ and $\bar{\mu} - \Delta$ should represent the intensity that would be observed at $\bar{\mu}$ in the absence of multiple diffraction.

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