# Short Communications

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## Parallel beams of neutrons or X-rays by multiple Bragg reflection.*

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A method of producing extremely parallel (and monochromatic) beams of neutrons or X-rays by multiple Bragg reflection in perfect crystals is proposed. The scheme is based on the simulation of a forbidden reflection by the cooperative action of three other reflections. The conditions necessary for obtaining the desired effect are discussed, and a short list of several reflections satisfying some of the conditions is given.

The purpose of this note is to point out the possibility of producing extremely parallel (and monochromatic) beams of neutrons or X-rays by multiple Bragg reflection in a perfect crystal. The proposed scheme is an extension of a previously described method in which a partially parallel beam is produced (Kottwitz, 1968). As in the earlier work the method is based on the simulation of a forbidden reflection by the cooperative action of other allowed reflections. However, instead of two cooperative reflections, there now must be three (or more). For simplicity we assume that there are only three.

A discussion of the necessary conditions is most readily carried out in terms of the kinematical (geometrical) theory and the reciprocal lattice (James, 1963). Let us consider four noncoplanar reciprocal-lattice points, the first of which is taken as origin (see Fig. 1). The four points are designated by their corresponding lattice vectors $\mathbf{h}_n$ ($n = 1, 2, 3, 4$). We note that the noncoplanarity condition may be expressed as

$$\mathbf{h}_2 . \mathbf{h}_3 \times \mathbf{h}_4 \neq 0 . \qquad (1)$$

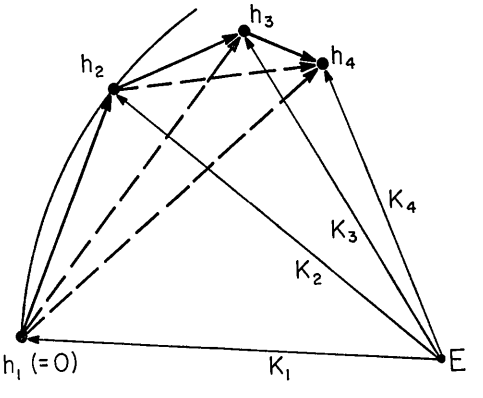


Fig. 1. An Ewald sphere (center $E$) passing through 4 noncoplanar points of the reciprocal lattice. Allowed reflections are shown by heavy solid lines, forbidden reflections by heavy dashed lines.

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It is known from geometry that there is a unique point $E$ (generally not a reciprocal-lattice point) equidistant from the four lattice points. We now construct an Ewald sphere with center $E$ and passing through all four lattice points. We assume that no other reciprocal-lattice points lie on the sphere. The four radius vectors $\mathbf{K}_n$ ($n = 1, 2, 3, 4$) represent the wave vectors of four plane waves that mutually diffract, one into another. We consider that $\mathbf{K}_1$ represents the incident beam and $\mathbf{K}_4$ the desired final diffracted beam.

It is clear from Fig. 1 that the incident $\mathbf{K}_1$ may be connected to the final $\mathbf{K}_4$ by a sequence of three reflections: $\mathbf{h}_2$, $(\mathbf{h}_3-\mathbf{h}_2)$, and $(\mathbf{h}_4-\mathbf{h}_3)$. Furthermore $\mathbf{K}_1$ and $\mathbf{K}_4$ are the only pair of wave vectors connected by this sequence. In general there are three other diffraction 'short cuts' from $\mathbf{K}_1$ to $\mathbf{K}_4$. These are the single direct reflection $\mathbf{h}_4$ and two sequences of two reflections: $\mathbf{h}_2$ and $(\mathbf{h}_4-\mathbf{h}_2)$, as well as $\mathbf{h}_3$ and $(\mathbf{h}_4-\mathbf{h}_3)$. However, if these three shortcuts are strictly forbidden by space-group symmetry, then the triple sequence of Bragg reflections stands alone and produces a final beam having a high degree of parallelism and monochromaticity (excluding multiple orders). Denoting the structure amplitude of a reflection by $F(\mathbf{h})$, we may write the necessary conditions as

$$F(\mathbf{h}_m-\mathbf{h}_n) \neq 0 , \quad m = n+1 , \qquad (2a)$$
$$F(\mathbf{h}_m-\mathbf{h}_n) = 0 , \quad m > n+1 . \qquad (2b)$$

In Fig. 1 the reciprocal-lattice vectors corresponding to the allowed reflections and forbidden reflections are shown by heavy solid and dashed lines, respectively.

In addition to equations (1) and (2) there are other conditions which must be satisfied in order that a triple Bragg reflection be useful for high-resolution collimation. If another simulation of the forbidden reflection $\mathbf{h}_4$ is nearby, it can spoil the triple reflection in the same manner in which double reflections are spoiled (Kottwitz, 1968). The interfering simulation may itself be either a double or triple Bragg reflection. A great amount of detailed calculation is required to resolve this question for each triple reflection.

Finally, there are two practical requirements that must be met. Sufficiently large and perfect specimens of the crystal must be available, and the absorption, inelastic and incoherent cross sections of its constituents must not be too large relative to the coherent, elastic cross section.

Table 1. *A sample of eligible triple Bragg reflections*

| Space group | Crystal system | Known crystals* | Forbidden $\mathbf{h}_4$ | Forbidden $\mathbf{h}_3$ | Forbidden $\mathbf{h}_4-\mathbf{h}_2$ | Allowed $\mathbf{h}_2$ | Allowed $\mathbf{h}_3-\mathbf{h}_2$ | Allowed $\mathbf{h}_4-\mathbf{h}_3$ |
|---|---|---|---|---|---|---|---|---|
| *Ia*3*d* | Cubic | 52 | 110 | 031 | 222 | $\bar{1}\bar{1}2$ | 143 | $1\bar{2}\bar{1}$ |
| *Fd*3*c* | Cubic | 2 | $00\bar{2}$ | 240 | 133 | $\bar{1}3\bar{5}$ | 375 | $\bar{2}4\bar{2}$ |
| *Pn*3*m* | Cubic | 10 | 012 | 201 | 120 | $\bar{1}\bar{1}2$ | $31\bar{1}$ | $\bar{2}11$ |
| *Pm*3*n* | Cubic | 24 | 111 | 122 | 001 | 110 | 012 | $0\bar{1}\bar{1}$ |
| *Pn*3*n* | Cubic | 0 | $0\bar{1}4$ | 100 | 131 | $\bar{1}4\bar{3}$ | $24\bar{3}$ | $\bar{1}\bar{1}4$ |
| *Pnma* | Orthorhombic | 402 | 012 | 021 | 100 | $\bar{1}12$ | $11\bar{1}$ | $0\bar{1}1$ |
| $P2_1/c$ | Monoclinic | 279 | 001 | 010 | 101 | $\bar{1}00$ | 110 | $0\bar{1}1$ |

* From Nowacki (1967).

Although no specific examples of potentially useful triple Bragg reflections are presently known, some progress has been made in narrowing the range of possibilities to be considered. The conditions on the structure amplitudes [equation (2)] are quite restrictive. Let us confine our attention to forbidden reflections that are forbidden strictly, that is, by virtue of space-group symmetry (*International Tables for X-ray Crystallography*, 1969). Then it is not difficult to show that only 5 space groups (of unfortunately infrequent occurrence) among the 10 belonging to class *m*3*m* of the cubic system can satisfy equation (2). Similarly, only 2 of the 8 most common (for inorganic crystals) space groups (Nowacki, 1967) are eligible. Unfortunately the cubic diamond structure (space group *Fd*3*m*) and the hexagonal close-packed structure (space group $P6_3/mmc$), both of which are suitable for double Bragg reflection (Kottwitz, 1968), are ruled out by the structure-amplitude conditions. For these 7 eligible space groups a limited amount of trial-and-error calculation has been done to find sets of reflections that satisfy equations (1) and (2). For each space group, a sample set of such reflections is given in Table 1, together with the crystal system and the number of known crystals (Nowacki, 1967).

### References

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## Polarization factor for graphite X-ray monochromators.

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Comparison of Ni-filtered and graphite-monochromatized Cu $K\alpha$ diffraction data indicates that the 'ideally imperfect' monochromator polarization factor is not applicable.

Since graphite was introduced as an X-ray monochromator the assumption of the polarization factor being that of an ideally imperfect crystal appears to have been tacitly accepted. A communication by Miyake & Togawa (1964), however, clearly points out that for high precision work it becomes necessary to test the validity of this assumption.

After a graphite monochromator had been installed on the Picker diffractometer in this laboratory part of the initial testing consisted of a comparison of a Cu $K\alpha$ (Ni filter) and a Cu $K\alpha$ (graphite monochromator) data set from the same crystal. For the comparison to be valid the specimen crystal must be perfectly stable towards X-ray irradiation, and secondary extinction effects must be small. A filter data set ($F_f$) satisfying these criteria was available from a reinvestigation of *p*,*p*′-dichloroazobenzene (initial study by Hope & Victor, 1969.) The structure had been refined to $R=0{\cdot}032$, with $|F_o|$ being about 5% smaller than $|F_c|$ for the most intense reflection. The crystal had been removed from the diffractometer with the goniometer head attached to the mounting base, and when the assembly was remounted on the goniostat it was found that the original setting parameters could be used without change.

The Cu $K\alpha$ (monochromator) data set was collected with exactly the same settings, scan ranges and background-count times as the filter data. About 950 reflections with $I_o > 2\sigma(I_o)$ which were common for the two data sets were used for comparison of polarization factors. The monochromator intensities were first reduced to *F*'s ($F_M$) by use of the polarization factor for an ideally imperfect monochromator with diffraction vector in a plane normal to the diffractometer equator, given by $p_K=(\cos^2 2\theta+\cos^2 2\theta_M)/(1+\cos^2 2\theta_M)$, where $\theta$ is the Bragg angle for the reflection under consideration and $\theta_M$ the monochromator Bragg angle (Azároff, 1955). [The corresponding expression for the 'perfect' monochromator is $p_D=(\cos^2 2\theta+|\cos 2\theta_M|)/(1+|\cos 2\theta_M|)$.]

Average normalized $F_M/F_f$ ratios were calculated for 5° ranges in $\theta$ with the results plotted in Fig. 1. Although small, the hump centered at $\theta=45°$ clearly points to a systematic, angle dependent error.

Following the procedure suggested by Miyake & Togawa (1964) the monochromator polarization factor was then expressed as $p=cp_D+(1-c)p_K$. From the shape of the initial $F_M/F_f$ curve a value of $c=0{\cdot}65$ was estimated, and a new set of $F_M$ was calculated. The average ratio was plotted as before, with the result also shown in Fig. 1. We see that above $\theta\sim35°$ the observed ratios very closely approach unity. At lower $\theta$ values there is a gradual drop to a ratio of 0·99 at 15°, pointing to some other systematic error. Inspection of the raw filter data revealed some degree of