Bioprocess Engineering and the Manners-Gandolfi *X*-ray Camera

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Abstract: *The purpose of this paper is to outline the mathematical design in the Manners X-ray camera in which a hypocycloidal gear system was used in order to avoid coincidences of planes in a certain type of X-ray crystallography.*

Keywords: *Bragg condition, Crystallography, Constructive interference, Hypocycloid, Monochromatic X-rays.*

Introduction

The powder diffraction technique is important in *X*-ray crystallography. In practice it is important to avoid coincidences of planes in fulfilling the Bragg condition for constructive interference of the incident radiation [1]. A number of methods have been developed to accomplish this [7, 8], but the method outlined here avoids the seemingly simple, but actually difficult, operation of re-placing the sample precisely in the holder of the Gandolfi camera.

Professors Terry Sabine and Tony Moon of the University of Technology, Sydney, identified difficulties in the ability of a Gandolfi camera to give a true picture of a triclinic crystal. The cause of this inefficiency in showing preferred orientation effects was the inadequacy of the randomising ability of the motion. Although this requires that the motion be unpredictable in the time-domain, its instantaneous vector must, of necessity, still be able to be described in terms of motion about and along the three co-ordinate axes with, hopefully, no predictable pattern of recurrences.

Vincent Manners approached the first author with a problem he was having in designing an *X*-ray diffraction camera to remedy these difficulties and which could rotate a sample about two generally normal axes while simultaneously rotating the sample about a third axis which would change in angular relationship relative to the two normal axes and also providing linear reciprocation of the sample along this third axis. Essentially the problem was to design an *X*-ray camera where the sample holder would oscillate through 90 degrees in the vertical plane while it continued to oscillate through 360 degrees in the horizontal plane and to avoid coincidences of crystal planes. This was achieved with a hypocycloidal gear mechanism [5] and the resulting device was patented [6] by the late Vince Manners, a former colleague of the authors.

The obvious theoretical solution of separate electric motors to control the oscillation and rotation was too complicated to implement in practice. What was desirable was a single driving mechanism to produce the two movements, while at the same time avoiding realignments of the same crystal planes.

The geometry of the hypocycloid

The hypocycloid, due to Girolamo Cardano (1501-1576), is the locus of a fixed point on the circumference of a circle rolling, without sliding, on the inside of the circumference of a larger circle. When the radius of the larger circle is double the radius of the smaller, inner, circle, then any point on the circumference of the latter follows a straight line which passes through the centre of the former; a diameter in other words. This provided a clue to an appropriate mechanism.

Let $P(x, y)$, originally at A, be the position of the tracing point when the contact of the circles has moved from A to H. Let R and r be the radii of the fixed and rolling circles respectively, and let θ and ϕ be the angles through which OH and CH respectively have turned (Fig. 1).

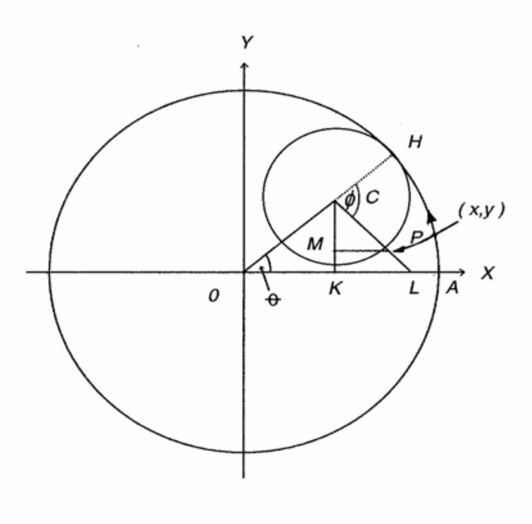

Fig. 1 Hypocycloid

We can then readily establish from this figure that the coordinates of P are

$$x = OK + MP = (R-r)\cos\theta + r\cos\left(\frac{R-r}{r}\right)\theta$$

and

$$y = KC - MC = (R-r)\sin\theta - r\sin\left(\frac{R-r}{r}\right)\theta$$

which reduces to $y = 0$ when $R = 2r$, and thus P traces out a straight line. This means that P can move up and down the x-axis, so that we can have the bottom of the sample holder fixed to this axis and the top fixed to the sample with an axle in between. A hypocycloidal gear mechanism was built so that when the Wheel 4 in Fig. 2 causes the Wheels 1 and 3 to rotate, the rod 2 moves up and down the slot 5. In this way if the rod is connected to the sample support, then the latter can oscillate in a rocking motion while the Wheel 1 rotates the sample holder.

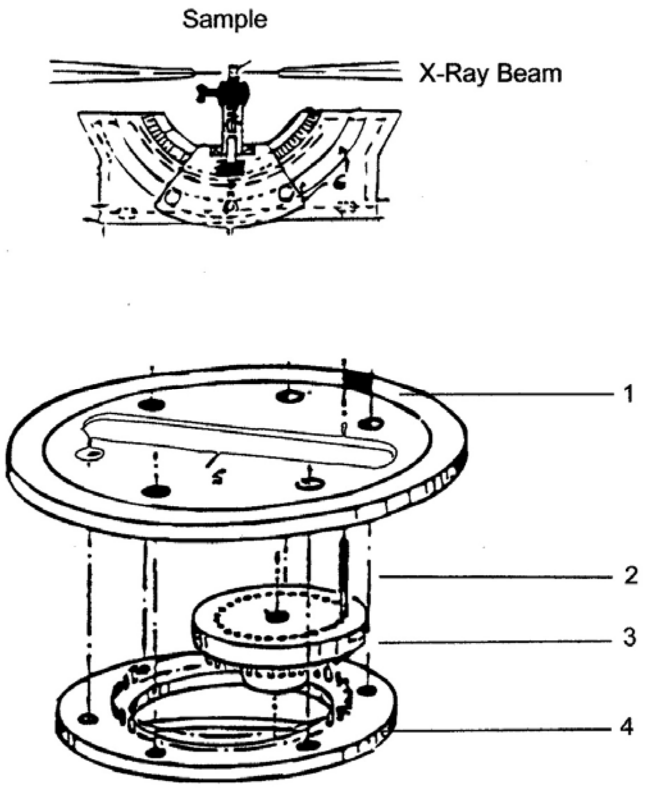

Fig. 2 Hypocycloid gear mechanism

The physics behind the problem

The essential feature of the powder diffraction technique is that a narrow beam of monochromatic *X*-rays impinges upon crystalline powder composed of fine, randomly oriented particles (as small as 0.1 µm (Fig. 3)). Ideally, all possible orientations of all possible planes are present so that the *X*-ray beam will always find some crystallites of the proper orientation to fulfil the Bragg condition for reflection.

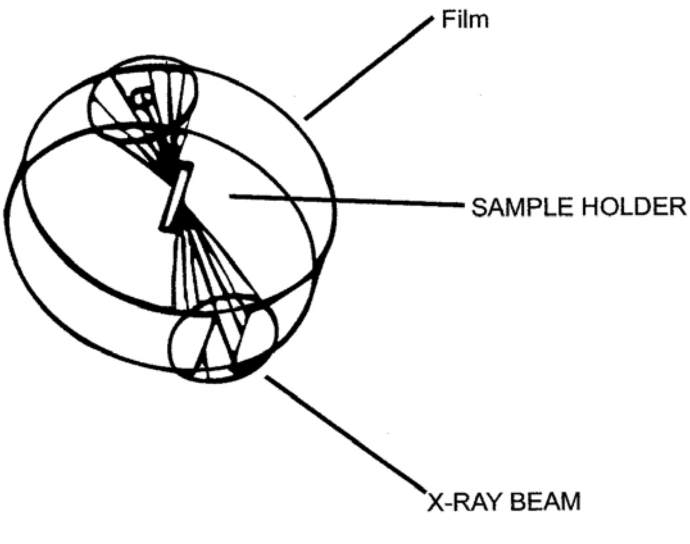

Fig. 3 Gandolfi camera

The Bragg condition for constructive interference of the incident radiation is given by

$$sin\psi = \frac{n\lambda}{2d},$$

where d is the distance between successive atomic planes in the crystal, λ is the wavelength of the radiation and n is an integer ($n = 1$ for a first order reflection). The variation in the angle ψ brings different planes into position of the objectives in the design of the Manners camera is to avoid coincidences of these planes (Fig. 4).

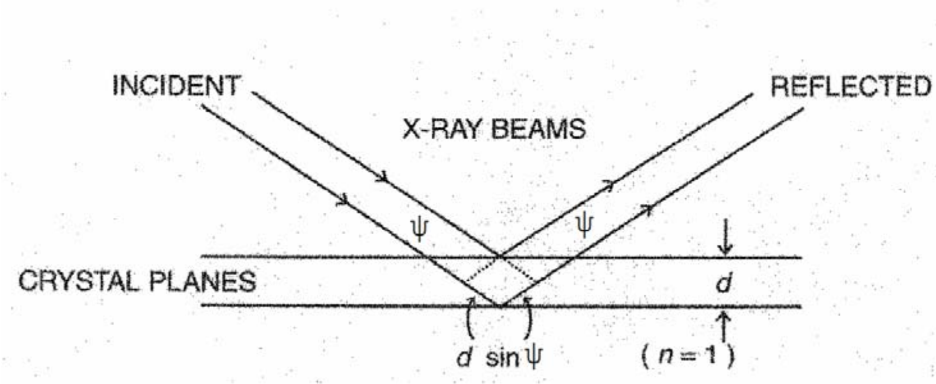

Fig. 4 The Bragg condition

The mechanism of the camera

As Wheel 2 rotates through angle θ, the base of the oscillating mechanism moves along the spherical surface from P' to P'_θ . That is, (Fig. 5):

- P': extreme position of oscillating mechanism;
- P'_θ : arbitrary position of oscillating mechanism;
- $2\pi/\dot{\phi}$: revolution time of end of rod;
- $2\pi/\dot{\theta}$: time taken for rod to traverse groove;
- S: sample (usually a small cylindrical holder filled with powder) is the centre of rotation of the rocking mechanism: $(-45^o < \alpha < 45^o)$ (Fig. 5).

Thus at P, $\tan 45^o = R/SP$, so that $SP = \sqrt{2}R$. Then P_θ lies on a sphere, centre S and radius $\sqrt{2}R$ with equation

$$x^2 + y^2 + z^2 = 2R^2.$$

In Fig. 1, Wheel 1 rotates with an angular velocity $\dot{\phi}$ relative to the small Wheel 2 which rolls inside Wheel 1 (rigidly attached to the base wheel) with an angular velocity of $\dot{\theta}$ relative to Wheel 2. This causes the rod to move to and fro along the groove, so that if P'_θ is the position of the rod after Wheel 2 has rotated through an angle θ (relative to Wheel 1), then P'_θ (x, y, z), a point on the surface of the sphere carved out by rod top when the small Wheel 2 rotates through angle θ relative to Wheel 1, is given by

$$x = R\cos\theta\cos\phi,$$
$$y = R\cos\theta\sin\phi.$$

From the equation of the sphere, we get

$$\begin{aligned}
2R^2 &= R^2\left(x^2 + y^2 + z^2\right) \\
&= R^2\left(cos^2\theta\, cos^2\phi + cos^2\theta\, sin^2\phi + z^2\right) \\
&= R^2\left(cos^2\theta\left(cos^2\phi + sin^2\phi\right) + z^2\right) \\
&= R^2\left(cos^2\theta + \left(2 - cos^2\theta\right)\right)
\end{aligned}$$

so that

$$z = R\sqrt{2-\cos^2\theta}.$$

That is, the *z*-value is independent of the rotation of Wheel 1 as required.

If we take h to be the thickness of the oscillating mechanism which is the same as the diameter of the cylindrical sample holder, then the area A swept out is the length of the arc times the thickness of the mechanism; that is,

$$A = hR\sqrt{2}\left(\frac{\pi}{4} - \alpha\right)$$

and so

$$\frac{dA}{dt} = -hR\sqrt{2}\,\frac{d\alpha}{dt}$$

$$\left|\frac{dA}{dt}\right| = hR\sqrt{2}\left|\frac{d\alpha}{dt}\right|.$$

In triangle OMP,

$$sin\,\alpha = \frac{MP}{SP} = \frac{z}{R\sqrt{2}}$$
$$z = R\sqrt{2}\,sin\,\alpha = R\sqrt{2 - cos^2\theta}$$
$$2\,sin^2\alpha = 2 - cos^2\theta$$
$$cos^2\theta = 2 - 2\,sin^2\alpha = 2\,cos^2\alpha$$
$$cos\,\theta = \sqrt{2}\,cos\,\alpha.$$

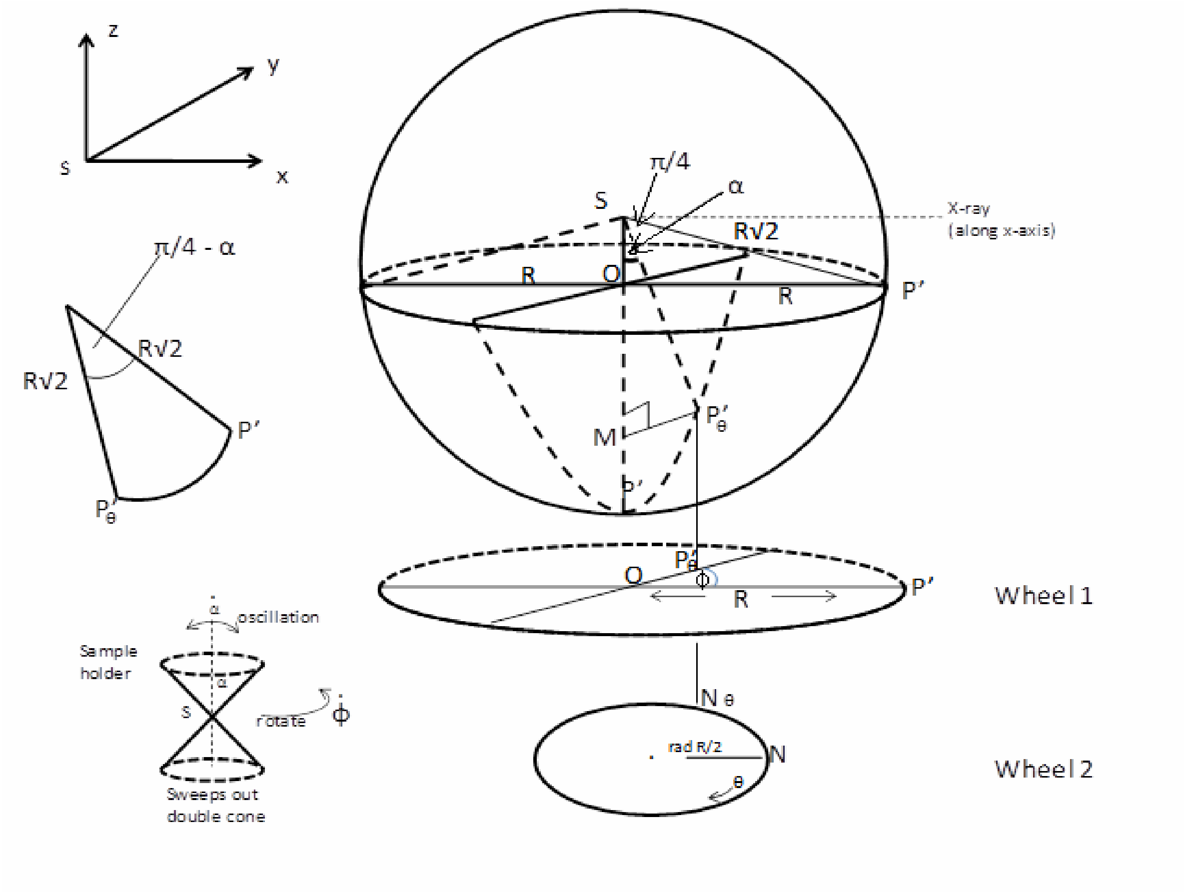

Fig. 5 Geometry of the mechanism

While an end point of the groove 5 of length $2R$ does one revolution in $2\pi/\dot{\phi}$ seconds, the rod 2 takes $2\pi/\dot{\theta}$ seconds to traverse the same groove. Coincidences will occur only when the rod is aligned above a position on the wheel that it has occupied previously and also when the wheel is simultaneously aligned with its starting point relative to the *X*-ray beam. This will occur only when integer multiples of the two angular velocities are equal: $m\dot{\theta} = n\dot{\phi}$. By choosing $(m, n) = 1$ with m a sufficiently large prime, we can, in principle, achieve our original purpose.

Conclusion

Sabine [9] has developed a complete mathematical treatment of the properties by which the reciprocal vector is aligned with the scattering vector. To further obviate any risks of alignment a piezo-electric crystal was used to provide electronic frequency generation in the direction of the *z*-axis and so give the holder movement in the third dimension [4].

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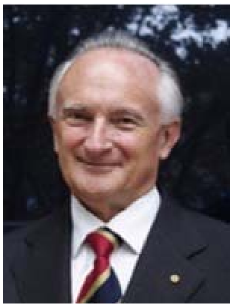

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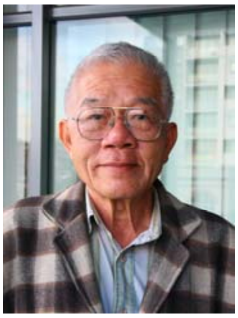

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