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A note on Burbank's paper on 'Intrinsic and systematic multiple diffraction'.

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Burbank (1965) has recently discussed under the title *Intrinsic and Systematic Multiple Diffraction* the conditions giving rise to multiple diffraction for the single-crystal orienter and for the precession camera. He concludes that there are important differences between the two techniques. For the single-crystal orienter, multiple diffraction will always occur if the crystal is mounted with a symmetry axis parallel to, or a symmetry plane normal to, the rotation axis (φ axis). For the precession camera, the conditions for multiple diffraction can be created or avoided at will by the choice of $\bar{\mu}$, regardless of crystal orientation. Burbank suggests that the zero-level precession technique is the only method in common use which offers the possibility of direct experimental observation of the magnitude of multiple diffraction effects.

The purpose of this note is to point out that there are no such differences between the two techniques if the orienter is used as a four-circle instrument with independent motion of the ω and 2θ axes. Although the original single-crystal orienter described by Furnas (1957) was a three-circle diffractometer, the majority of instruments commercially available today have four independent axes: the direct experimental observation of multiple diffraction with these four-circle instruments has been fully described by Willis (1962) and by Santoro & Zocchi (1964). The situation discussed by Burbank corresponds to the use of the orienter as a three-circle instrument, with the angle ε between the χ plane and the normal to the *hkl* plane under observation as zero. This $\varepsilon=0$ (or 'symmetrical *A*') setting is formally equivalent to the equi-inclination Weissenberg setting (Phillips, 1964) and gives rise, therefore, as Burbank shows in another way, to multiple diffraction under the same conditions as for the equi-inclination setting (Yakel & Fankuchen, 1962).

The limitation of Burbank's analysis to the $\varepsilon=0$ setting is apparent in his answer to the question: Is there a reciprocal lattice plane coincident with the vertical circle of reflexion? Burbank states that, 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 reflexion. This is true only if the φ axis is in the plane of the vertical circle of reflexion. The φ axis is mechanically constrained to lie in the vertical χ plane, and the vertical circle of reflexion and the vertical χ plane are in coincidence for $\varepsilon=0$ but not in the general case, $\varepsilon\neq 0$.

The essential *similarity* of the precession and single-crystal orienter techniques as regards observing multiple diffraction effects is strikingly illustrated by reference to the last section of Burbank's paper. The procedure described there for creating or avoiding at will multiple diffraction with the precession technique is exactly paralleled for the orienter technique. If a symmetry axis of the crystal is parallel to the φ axis of the orienter, the *hkl* intensity is first recorded with a zero off-set angle ε, corresponding to the condition for intrinsic multiple diffraction. ε is then given a small increment, positive or negative, sufficient to destroy the multiple diffraction condition, and the intensity re-measured. Any difference in the two intensities is due to multiple diffraction.

References

Burbank, R. D. (1965). *Acta Cryst.* **19**, 957.
Phillips, D. C. (1964). *J. Sci. Instrum.* **41**, 123.
Santoro, A. & Zocchi, M. (1964). **17**, 597.
Willis, B. T. M. (1962). *Brit. J. Appl. Phys.* **13**, 548.
Yakel, H. L. & Fankuchen, I. (1962). *Acta Cryst.* **15**, 1188.

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Disorder in erythrocyte catalase crystals.

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Introduction

Catalase is an enzyme which decomposes hydrogen peroxide into oxygen and water. It consists of protein, combined with four haem groups, and has a molecular weight of 238,000, as calculated from the sedimentation constant and iron content (Lamberg & Legge, 1949).

The catalase crystals

Horse erythrocyte catalase was crystallized according to Bonnichsen (1947). Crystals grew in two to three weeks in

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