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Design for a Goniometer Head

BY D. A. DAVIES AND A. McL. MATHIESON
Chemical Physics Division, C.S.I.R.O. Chemical Research Laboratories, Melbourne, Australia

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From consideration of the basic operations of a three-circle goniometer, practical designs for goniometer heads are derived. An alternative to the design now standard for 35 years is indicated. Some factors with respect to this design are investigated and methods of its application to the alignment of a crystal axis outlined.

The design of the new goniometer head was stimulated by the need, in optical grating manufacture, for a device to set a diamond at a specific orientation in which it would be held for grinding, conditions which placed considerable emphasis on rigid construction.

A goniometer head with its supporting shaft is, in essentials, a three-circle goniometer with restricted ranges of the two angular variables χ, φ to permit limited adjustment of a crystal axis to parallelism with the main rotation axis, ω, of the unit. Consideration of the basic design of a three-circle device (Fig. 1(*a*)) indicates possible ranges of operation most suitable to the design of a goniometer head. With the φ circle located near $\chi=270°$ (or 90°) (Fig. 1(*b*)) variation of $\varphi \pm 30°$ around $\varphi=0°$ and of $\chi \pm 30°$ around $\chi=270°$ can be used for the purposes of adjustment. This choice for the operational ranges of φ and χ can be recognized as the mode of operation of the standard goniometer head (Fig. 2, left). For reasons of compactness and simplicity of construction, this configuration is conventionally achieved by utilization of an arc of limited extent at *A* (Fig. 1(*b*)) which replaces the physical axis of φ at $\chi=270°$. Although almost universally used for single-crystal studies for the last 35 years, this is not the only possible arrangement satisfying the basic requirements of a goniometer head. An alternative mode of operation for crystal axis alignment is to locate the φ circle axis near $\chi=0°$ (Fig. 1(*c*)) with provision for a $\sim 30°$ range of adjustment of χ and a full 360° adjustment of φ. This configuration still fulfils the requirement that the physical variable be located in the region of *A* (Fig. 1(*c*)). This alternative design is realized in an *ad hoc* manner in Fig. 2 (right).

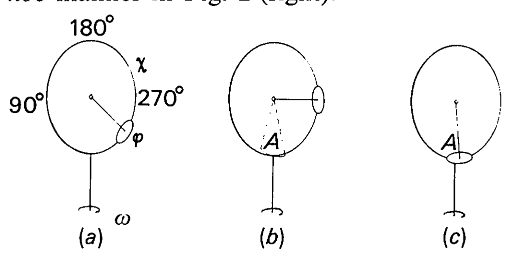


Fig. 1. (*a*) Schematic diagram of a three-circle device detailing variables χ, φ and ω. (*b*) Configuration of the earlier goniometer head design, effective φ circle axis at $\chi=270°$ with limited range of φ near $\varphi=0$, equivalent to arc at *A*. (*c*) Configuration of the new design with the φ circle adjacent to $\varphi=0°$.

The goniometer head

In terms of their function of orienting a crystal axis in space, the old and new goniometer heads are equivalent and equally suitable. Comparison of possible relative advantages and disadvantages must depend on factors which are determined by its specific usage— such as simplicity of construction and inherent accuracy, the physical compactness of the design and ease of adjustment.

The fabrication of accurate arcs is not an easy matter and the end-result is not particularly precise by comparison with complete circles (*e.g.* Wooster, 1963). From this viewpoint, it is therefore to be regarded as advantageous that the new design requires only one arc. Since the φ circle performs a complete rotation, it can be mounted on stout bearings. By contrast, the standard design involves two arcs, one mounted upon the other so that their individual inaccuracies are compounded (Fig. 2, left). The new design should therefore be inherently rather more robust and less liable to errors arising from deflexions of its parts.

From the viewpoint of compactness, *i.e.* with respect to obstruction of beam stop, collimator, layer-line screens *etc.*, the present model, built only to test the design, cannot give a complete assessment of its inherent capabilities, but it provides a guide. Fig. 2 (right) suggests that the new design could be more compact and obtrude less than the old design.

The problem of adjustment with the new goniometer head to align a crystal axis cannot be answered by a direct reference to the literature on the two-arc goniometer head since the variables are more conveniently assessed by a slightly different approach dealt with in the following section. This discussion is based on the use of film as detector but may prove useful as a guide towards setting with a quantum counter.

Modes of adjustment

For goniometer heads, adjustment of a crystal axis only within a limited angular range is involved and therefore the more complete discussion relating to three-circle devices with complete circles (*e.g.* Willis, 1961, 1962; Wooster & Wooster, 1962) is not required. Since the angular range of operation is restricted, it is possible to recognize comparative relations between the

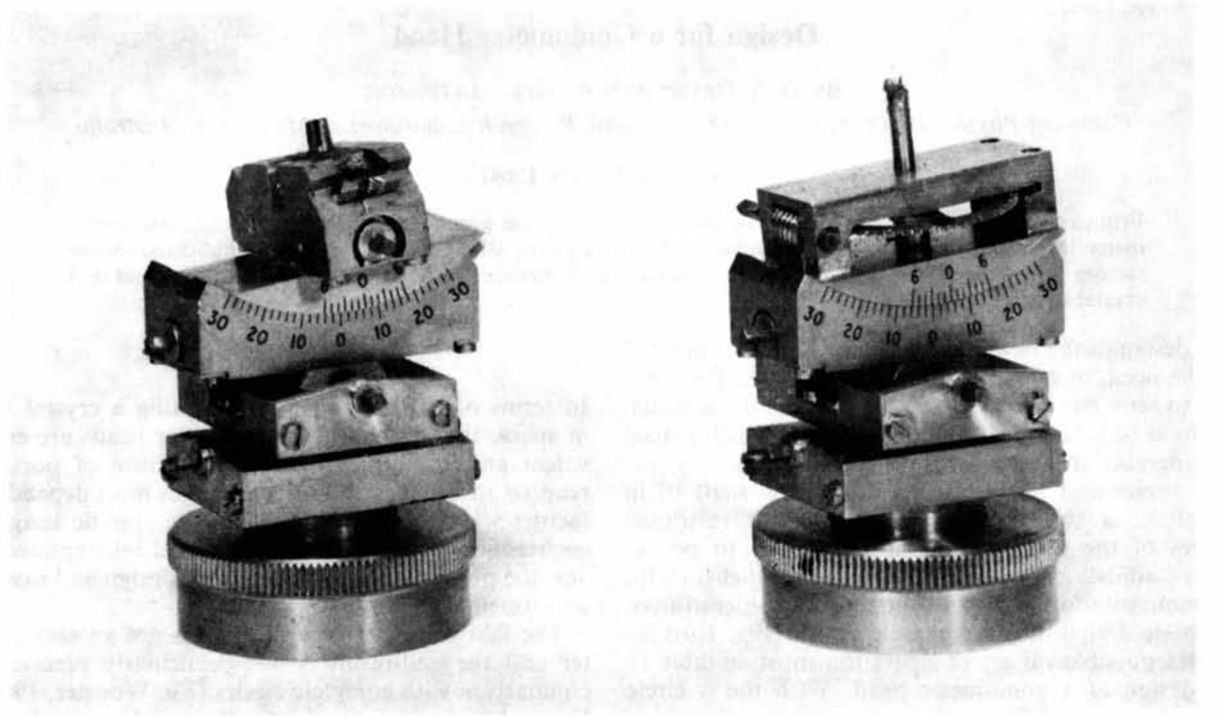
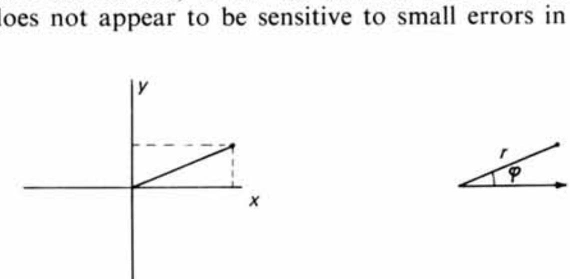


Fig. 2. Left: the two-arc gonoimeter head corresponding to Fig. 1(*b*). Right: the one-arc head corresponding to Fig. 1(*c*).

old and new designs which can be of use in approaching the problem of setting. Thus the two-arc design may be considered as based on independent rectilinear coordinates x, y (Fig. 3(*a*)) with $x \equiv \chi$ at 0° and $y \equiv \varphi$ at 270° whereas the new design is most naturally treated in terms of polar coordinates r, Φ (Fig. 3(*b*)) where $r \equiv \chi$ at 0° and $\Phi \equiv \varphi$.

The mode of setting for the new goniometer head must be such as to determine $\Delta r (\equiv \Delta\chi)$ and $\Delta\Phi (\equiv \Delta\varphi)$ and these are not readily determined independently. Before adjustment of r can be made, Φ must be rotated to $\Phi = 0°$ so that Δr is then parallel to the χ arc. Hence it is necessary to determine in which quadrant Φ lies and also the magnitude of r.

One mode of operation could be to record double exposures (*i.e.* $\omega = 0°$ and 180°) with the X-ray beam parallel to the arc (Fig. 4(*a*)) and then with the beam perpendicular to the arc (*i.e.* $\omega = 90°$ and 270°) (Fig. 4(*b*)). From the slopes and displacements of the zero-layer at or near $2\theta = 0°$ and 180° respectively, corrections $\Delta\Phi$ and $\Delta r (\equiv \Delta\chi)$ can be deduced in a manner similar to that recorded in Bunn (1945), with the utilization of correction procedures analogous to those of Kratky & Krebs (1936), of Hendershot (1937) and of Weisz & Cole (1948). A variant to this procedure is to carry out a double exposure with the arc at 45° to the X-ray beam (*i.e.* $\omega = 45°$ and 225°). By this method, the component of the correction parallel to the arc, $\Delta r \cos \Phi$, would be determined. After this correction is effected, Φ could be rotated through 90° and the rectilinear component, $\Delta r \sin \Phi$, now parallel to the arc, could be determined by a double exposure, also at $\omega = 45°$ and 225°. However the simplest procedure arises from the method just discussed and is essentially Davies's (1950) method, applied to the one-arc goniometer head. With the arc set at 45° to the main beam, a double exposure ($\omega = 45°$ and 225°) is recorded. The components $\Delta_L = \Delta r \cos \Phi$ and $\Delta_R = \Delta r \sin \Phi$ are recorded on left-hand ($2\theta = -90°$) and right-hand ($2\theta = +90°$) sides of the film (Fig. 5). From this one film, the two components are derived and the individual corrections for r, $\Delta r = (\Delta_L^2 + \Delta_R^2)^{\frac{1}{2}}$ and Φ, $\Delta\Phi = \tan^{-1} \Delta_R / \Delta_L$ determined, the relation of the magnitude of the correction to the radius of the film being as given by Davies (1950). From the relation of Φ to the component corrections, it will be obvious that the setting does not appear to be sensitive to small errors in Φ.



(*a*) (*b*)

Fig. 3. The variables used in setting (*a*) the two-arc head and (*b*) the one-arc head.

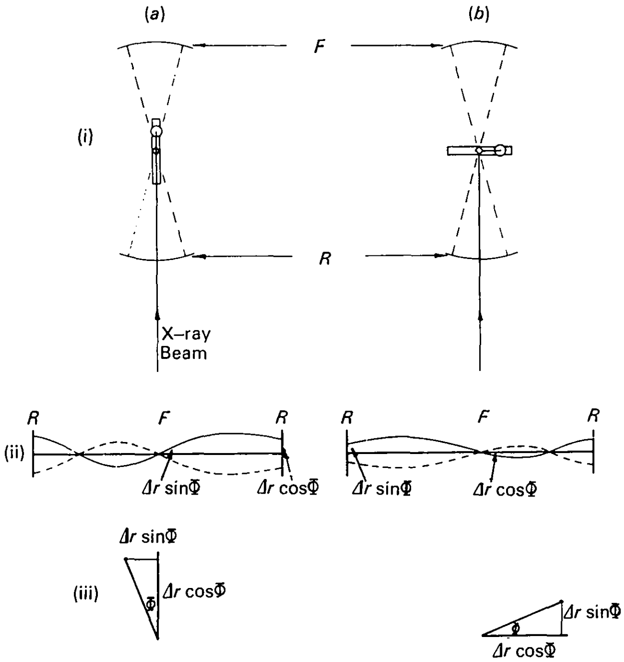


Fig. 4. Method of determining the component corrections $\Delta r \cos\Phi$ and $\Delta r \sin\Phi$ by alignment of the arc (*a*) parallel and (*b*) perpendicular to the X-ray beam. *F* and *R* the are forward and rear portions of the film. (i) corresponds to the view down the ω axis. (ii) the trace of the two exposures of the zero-layer on film, and (iii) the orientation of the components as viewed down the ω axis.

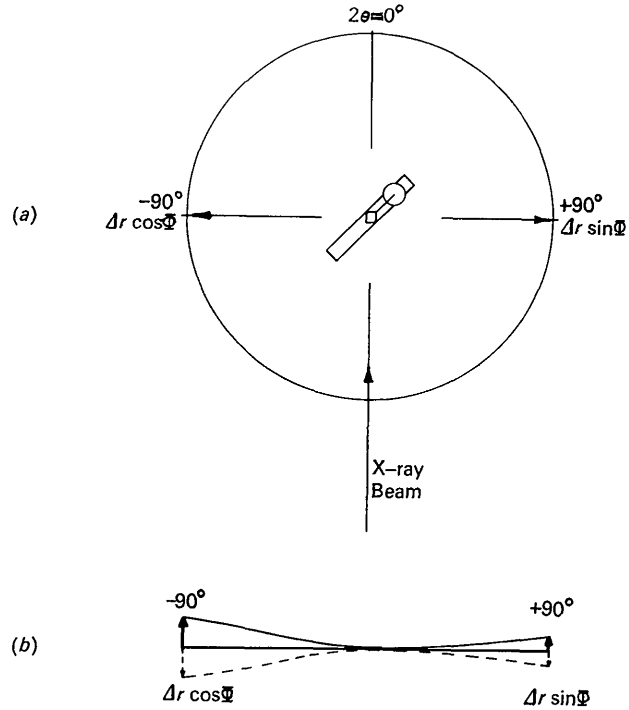


Fig. 5. Determination of the component corrections with the arc at $\omega = 45°$ and 225°. (*a*) Disposition of the X-ray beam and film as viewed down the ω axis. (*b*) The components as viewed on the film, $\propto \Delta r \sin\Phi$ and $\propto \Delta r \cos\Phi$ at $2\theta = +90°$ and $-90°$ respectively.

Conclusion

The discussion on alignment with an r, Φ goniometer head using film as detection medium may be found useful in the initial adjustment of its more elaborate relations—the Eulerian cradle (Furnas & Harker, 1955) and the three-circle goniometer (Willis, 1961; Wooster & Wooster, 1961; Arndt & Willis, 1963). The present discussion may provide a rationale for the initial setting of crystals in two- and three-circle devices which is rather different in approach from that developed by Furnas (1957) based on a search of reciprocal space with a counter. The incorporation of a simple film-holder for initial settings on a multi-circle device would appear to be advantageous.

It is of interest to note that the viewpoint developed here of a goniometer head as a three-circle goniometer with limited angular adjustment stresses the redundant role which a goniometer head plays in a three-circle goniometer. For such instruments, the basic requirement is a device to permit centring (Ladell, 1963) since initial adjustment of a crystal axis to a particular orientation can be completely handled by the two variables χ, φ (Fig. 1(*a*)). Once set to χ_0, φ_0 these become the reference origins in the system of angular variables.

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