Letter to the Editor

J. Appl. Cryst. (1984). **17**, 369

Recommendations of the *Ad hoc* Committee on Criteria for Publication of Charge Density Studies*

Sir,

The Committee is of the firm opinion that guidelines should not attempt to prescribe how crystallographic research is to be performed. This is strictly the prerogative of the individual investigator. Also, optimal experimental methodology will vary with time, with available facilities, and with the aims of the research.

However, a manuscript should provide the requisite information to allow referees and readers to make an informed judgment about the reliability of the reported conclusions. The amount of detail provided for this purpose should be consonant with the significance explicitly or implicitly claimed for the results presented. The following information, much of which is probably desirable in any crystallographic study claiming high accuracy, should normally be regarded as a near minimum requirement in any publication reporting quantitative charge density results.

1. A full description of basic experimental procedures, such as preparation and testing of crystal specimens, temperature control, incident radiation, scan parameters, monitoring, background determination, *etc.*

2. How systematic errors such as absorption, extinction, scan truncation and the like were corrected, or why such effects were considered unimportant.

3. The method used for estimating the variances of the measured structure amplitudes.

4. Internal consistency indices if symmetry-equivalent reflections were measured.

5. Evidence for the compatibility of X-ray and neutron data if both were used together, particularly with regard to crystal quality and temperature.

6. The method for scaling X-ray data in the calculation of *X–X* or *X–N* maps.

7. Complete listing of (anisotropic) atomic vibration parameters, at least for non-hydrogen atoms.

8. Representative residual density maps, or summary descriptions thereof, after the highest level of refinement reported, the required number of such maps depending on the complexity of the structure.

9. An estimate of the expected error in deformation densities and in derived quantities, with an explanation of how the errors were estimated.

10. Lists of the experimental structure amplitudes and their statistical weights should be available to the referees and submitted for deposition.

11. If theoretical calculations are reported, the nature of all approximations, basis sets, *etc.* should be fully specified. Contour intervals in experimental and theoretical maps should be readily comparable.

*Committee appointed by the Commission on Journals on 26 April 1983.

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Laboratory Notes

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A sample holder for cutting single crystals along any desired X-ray oriented plane

Recently, a device has been reported (Campos, Cardoso & Caticha-Ellis, 1983) for cutting single crystals to any desired orientation to a high accuracy. We report in this note a very simple jig for a similar purpose, which can be easily fabricated in an ordinary laboratory workshop. The method employed can be used when only moderate accuracy is desired and is suitable specifically for long metal crystal rods. The crystal can be fixed on this jig, removed from the X-ray goniometer and easily transferred to a cutting device without disturbing its orientation set by X-ray goniometry. The jig described here has been designed for a Unicam goniometer; however, suitable alterations can be made for other types.

The jig has, as its base, an annular ring *B* (Fig. 1), which can be freely accommodated in the central circular housing of the goniometer. Two flat vertical supports, *S*, of rectangular shape are welded to this base at diametrically opposite ends and at right angles to the base plane. A rectangular flat frame, *F*, with horizontal *V* grooves in its longer sides is fitted to the top of these supports. The frame carries a pair of plates, *P*, having *V* cuts at their inner centres and sliding along their edges in the *V* grooves. The plane of these plates is made flush to the plane of the frame. Sliding motion of the plates is achieved by long screws, *T*, passed through the centres of the shorter sides of the frame and fixed to the plates. One of the flat supports of the jig is provided with a hole to fix the jig to the pedestal of the cutting wheel by a bolt. The complete jig is made of brass and weighs about 1·3 kg, providing good stability.

To use this jig, the crystal is first X-ray oriented on the goniometer so as to make the desired plane horizontal (*e.g.* as shown by the dashed section in Fig. 1). The jig is then placed over the oriented crystal on the goniometer and the sliders are slowly pushed inward until they just touch the crystal surface. The crystal is then stuck to the jig by good-quality resinous glue. Once the glue has set, the crystal is carefully freed from the goniometer head. The jig, carrying the crystal, is then removed for the cutting.

The jig is placed flat on its side on the pedestal of a diamond cutting wheel and fixed with a nut and bolt as shown in Fig. 2. This makes the required crystal

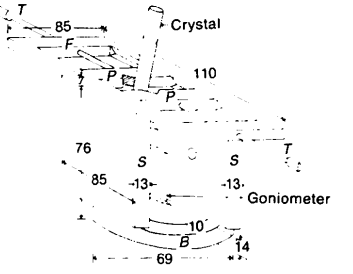

Fig. 1. Schematic diagram of the sample holder (all dimensions in mm).

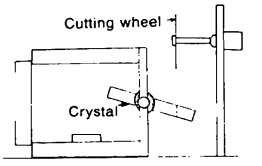

Fig. 2. Positioning of the sample holder and cutting wheel.

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