

For standard simple constraints Rietveld's program including Lagrange undetermined multipliers is superior as such constraints are included in his basic program. With modest experience it is easy to write the subroutine for most such constraints, but as the possibility of using Lagrange's method may in certain cases be essential this facility has been included in *EDINP* in a rudimentary manner. More details are given in the program description prepared for users.

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Laboratory Notes

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A fast and accurate way of aligning X-ray cameras

With only a fluorescent screen and a needle mounted on a goniometer head, it is possible to adjust the X-ray beam relative to the axis of rotation to within about 10 μm .

The axis of rotation of most X-ray cameras (such as Weissenberg, precession and rotation cameras) is perpendicular to the X-ray beam. If the center of the X-ray beam does not coincide very accurately with the axis of rotation of the camera, the X-rays illuminating the crystal will be of different intensity at different settings of the spindle. This is a problem especially when very small crystals and fine collimators are used, in which case there is even a risk that the X-rays completely miss the crystal. It is then essential to be able to adjust the X-ray beam to coincide within a few micrometers with the axis of rotation. On many X-ray cameras this adjustment is very tedious. With the method presented here, the alignment of the camera can be checked very easily, and any deviation from perfect alignment will be detected in a quantitative and accurate way.

A needle is mounted on a goniometer head and made to coincide with the axis of rotation. The needle is then translated along the axis of rotation until the tip of the needle intersects the direct beam. The needle is then translated s mm in a direction perpendicular to the axis of rotation, e.g. 1.0 mm. The exact length of the translation should be measured using the microscope on the camera. This is most easily done if the microscope is equipped with a scale which is calibrated

with a ruler held at the crystal position. If the spindle is rotated, the needle will intersect the direct beam twice per 360°. If the axis of rotation and the direct beam coincide exactly, the two readings (ω_1 and ω_2) on the spindle will be 180° apart. If, however, the two axes do not coincide, the needle will intersect the direct beam at two readings on the spindle which are not 180° apart, e.g. 280 and 80°. The angular position of the spindle can be accurately determined just by looking at the direct beam hitting a fluorescent screen, while rotating the spindle and noting when the shadow of the needle is seen. This information is sufficient to determine how far (d mm) the two axes are from intersecting each other, as seen in Fig. 1: $d = s \sin [(\omega_1 - \omega_2 - 180)/2]$.

If s is 1.0 mm, $\omega_1 = 280$ and $\omega_2 = 80^\circ$, d becomes $1 \times \sin 10^\circ$, i.e. 174 μm . By repeating the procedure with smaller or larger offsets of the needle, it becomes evident that this method is very accurate, and the distance between the two axes can easily be determined to within 10 μm . This is more than ten times the accuracy that can be achieved by taking pictures of the shadow of the needle in the direct beam. Also, the method suggested here is much faster, as there is no need for

developing films. After readjusting the height of the collimator relative to the axis of rotation the measurement is repeated until the desired accuracy is achieved. Finally, the point of intersection along the rotation axis is determined by looking through the microscope at the image of the direct beam on the fluorescent screen.

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Reliable temperature readings in the low-temperature Guinier–Lenné camera

We redesigned the cold finger of a Guinier–Lenné powder camera (Enraf–Nonius, Delft; see de Jonge, Popma, Wiegers & Jellinek, 1970). The new design guarantees a temperature reading correct to within 2 K, while the temperature differences within the sample are reduced to at most a few tenths of a degree.

The original cold finger consisted of a thermal flow resistance, a heating element and a sample compartment. It gave temperature readings which we sometimes found to be some 40 K in error. We

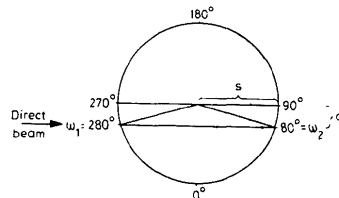


Fig. 1. The correlation between the angular readings (ω_1 and ω_2) on the spindle and the distance (d) between the axis of rotation and the direct beam of an X-ray camera.