The Asymmetrically Cut Bonse–Hart X-ray Diffractometer.
II. Comparison with the Kratky Camera*

BY MOSHE DEUTSCH
Department of Physics, Bar-Ilan University, Ramat-Gan, Israel

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Abstract
The asymmetrically cut, optimized BH diffractometer for small-angle X-ray scattering experiments is compared with the Kratky camera. It is shown that a crossover point exists in the resolution so that at a lower resolution the Kratky camera is superior and at a higher resolution the BH system is preferable. The crossover point depends on the number of reflections used. Methods of reducing the spurious signal and increasing the S/N ratio of the BH system are also discussed.

Introduction
In a previous paper (Deutsch, 1980), the design principles of asymmetrically cut Bonse–Hart (BH) diffractometers for small-angle X-ray scattering measurements were presented. A method was developed for optimizing the performance of the diffractometer so as to obtain the highest intensity allowed by (i) the required resolution, and (ii) the spurious signal which can be tolerated. In this paper we compare the performance of the optimized BH diffractometer with that of a widely used small-angle X-ray diffractometer based on slit focusing optics: the Kratky camera (Kratky, 1954, 1958; Kratky & Skala, 1958; Kratky & Leopold, 1964; Stabinger & Kratky, 1979).

In the next section the theory of the Kratky camera and some results derived for the asymmetric BH diffractometer are reviewed. The third section is devoted to a detailed comparison of the resolution, intensity and S/N ratio obtainable with the two systems.

Theory
(a) The Kratky camera
This device employs geometrical focusing by means of a set of blocks to obtain a well collimated primary beam with a very low level of parasitic scattering. The geometry of the camera is given in Fig. 1. The angular divergence of the primary beam is

\[ \Delta_{1K} = \epsilon / a \]  

(1)

and the intensity \( P_K \) at the sample, if the entrance slit is fully illuminated, is given by (Kratky & Leopold, 1970)

\[ P_K = ce^2 / 4a = (c/4)e\Delta_{1K} \, . \]  

(2)

where \( \epsilon \) is the width of the entrance slit, \( a \) is the half-length of the collimating system and \( c \) is some constant, the value of which depends on the X-ray source. It can be shown that for maximum intensity at a given resolution the width \( z \) of the measuring slit must be half that of the primary beam at the plane of registration (Kratky & Leopold, 1970). Thus,

\[ z = \epsilon (a + b + r) / 2a \, . \]  

(3)

The divergence of the scattered beam is

\[ \Delta_{2K} = z / r = \epsilon (a + b + r) / 2ar \]

and the intensity \( I_K \) measured is

\[ I_K = P_K \delta \Delta_{2K} = c'e^{3}(a + b + r)/8a^2r \, . \]  

(4)

where \( c' = c\delta \) and \( \delta \) is the scattering power of the sample. Thus, there is an explicit relation between the angular divergences of the primary and scattered beams and the measured intensity

\[ I_K = (c'/4)e\Delta_{1K}\Delta_{2K} \, . \]

(b) The BH diffractometer
Here the primary beam is collimated by successive Bragg reflections in a grooved crystal (Bonse & Hart, 1965, 1966a,b). The primary beam intensity is propor-

Fig. 1. Kratky-camera geometry. F is the line source, S is the sample, R is the plane of registration, \( \epsilon \) is the entrance-slit width and \( z \) the measuring-slit width. The dimensions are: \( a = 60, b = 20, r = 220 \) mm. Note that the vertical dimensions are greatly enlarged relative to the horizontal ones.

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tional to the integrated intensity and the angular divergence of the primary beam is given by the FWHM of the effective reflection curve. Thus,

$$P_{BH} = cdQ_{BH},$$

where \( Q_{1BH} \) is the integrated intensity of a crystal cut at an angle \( \alpha_1 \) so that the FWHM of its reflection curve is \( \Delta_{1BH} \). \( d \) is the apparent width of the line source and \( c \) is the same as in (2). The measured intensity is given by

$$I_{BH} = P_{BH} Q_{2BH} = c' dQ_{1BH} Q_{2BH},$$

(5)

where \( c' \) is the same as in (4) and \( Q_{2BH} \) is the integrated intensity of the analysing (second) crystal which is cut at an angle \( \alpha_2 \) such that the FWHM of its reflection curve is \( \Delta_{2BH} \). Note that here no explicit relation can be written between the divergences of the primary and scattered beams and the intensity since no such relation exists between the width and the integrated intensity of the reflection curve.

**Discussion**

The equations given in the previous section can be used to compare the performance of the two systems. We have chosen to do the calculations for the block system used by Kratky & Leopold (1970) in their comparative study of the Kratky camera and the original, symmetric Bonse–Hart system. The numerical values of the various parameters are given in Fig. 1. The BH diffractometer is the 111-reflection Ge perfect-crystal type discussed by Deutsch (1980).

As the entrance slit of the Kratky camera is opened, the measuring-slit width \( z \) must also be increased to preserve the relation given in (3). Thus, with increasing \( e \) both \( \Delta_{1K} \) and \( \Delta_{2K} \) increase linearly, while the measured intensity increases as the third power of \( e \). The asymmetric BH diffractometer equivalent to the Kratky camera with a given \( e \) is the one having the same resolution in both the primary and scattered beams; that is

$$\Delta_{1K} = \Delta_{1BH},$$

$$\Delta_{2K} = \Delta_{2BH},$$

(6)

which implies different values of \( \alpha \) for the collimating and analysing crystals. We have calculated \( I_{K} \) and \( I_{BH} \) according to (4) and (5) as a function of \( e \) using the parameters given in Fig. 1 and the restrictions given in (6). The results are given in Fig. 2 for one, two and four reflections off the (111) planes of Ge in each grooved crystal. As expected, at high enough resolution the asymmetrically cut BH system is superior to the Kratky camera: for \( e = 10 \mu m \) the equivalent BH system yields a 22-, 44-, and 84-fold increase in the intensity over the Kratky camera for the four-, two- and one-reflection cases, respectively.

The peaking effect (Deutsch, 1980) can be seen clearly in Fig. 2. Thus, for example, it is clear that the four-reflection BH diffractometer equivalent to the \( e = 15 \mu m \) Kratky camera yields the highest intensity obtainable with four reflections. Moreover, this intensity is higher than that of the Kratky system with any \( e \) less than 30 \( \mu m \). Fig. 2, therefore, predicts a crossover point for the asymmetric BH diffractometer under consideration. If resolution and S/N considerations dictate the use of either a Kratky camera with some value of \( e \) less than 30 \( \mu m \) or a BH system with four reflections, the latter choice is to be preferred since it yields higher intensity, whereas if \( e \) greater than 30 \( \mu m \) is required, the Kratky camera is to be used. Moreover, if the BH system corresponding to some \( e \) in the range 15 to 30 \( \mu m \) is chosen, the peaking effect dictates that actually a BH device equivalent to \( e = 15 \mu m \) has to be used since it yields higher intensity in spite of its too high resolution. For the two-reflection case, the crossover point is \( e = 54 \mu m \) and the peaking is less pronounced, while for the one-reflection case the crossover is at \( e = 125 \mu m \) and no peaking exists.

The question of the S/N ratio and the spurious signal of the BH diffractometer has already been discussed (Deutsch, 1980). Excluding the wings of the reflection curve (which are in any case minimized by choosing the right number of reflections for each BH diffractometer), we find that the main source of noise is the thermal diffuse scattering. This can be greatly reduced by trapping the main beam in front of the analysing crystal and using a pair of parasitic scatter slits at the point where the primary beam emerges from the collimating crystal. Thus, the large parasitic scattering measured by Kratky & Leopold (1970) for the symmetric BH collimator seem to have been measured without using

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Fig. 2. Intensity obtained from an asymmetrically cut BH diffractometer and the equivalent Kratky camera. The horizontal and vertical dashed lines indicate the crossover points. --- BH one reflection; — BH two reflections; ---- BH four reflections; —- Kratky camera.
the two contraptions mentioned above. Moreover, the thermal diffuse scattering is independent of $\alpha$ so that about the same parasitic scattering is expected for the asymmetric case as measured for the symmetric one, while the intensity is now increased by at least one order of magnitude. Thus, a significant increase in the S/N ratio is obtained in the asymmetric case relative to the symmetric one.

**Conclusion**

We have shown that a crossover point exists for the resolution above which the asymmetric BH diffractometer yields an intensity in some cases two orders of magnitude higher than the Kratky camera. For resolutions lower than that, the Kratky camera is superior to the asymmetric BH system. As the number of reflections in the grooved crystal is changed, the crossover point assumes different values. It was also shown that by taking some precautionary steps, the spurious signal in the BH system can be greatly reduced. This, and the increase in the signal due to the asymmetry will give a much higher S/N ratio than that measured by Kratky & Leopold (1970) for the symmetric BH diffractometer.

**References**