



JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

Volume 54 (2021)

Supporting information for article:

Multipurpose diffractometer for in-situ X-ray crystallography of functional materials

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We measured the geometrical beam divergence by “photographing” the beam image (as in Figure 3a) at several detector distances (D). The non-overlapping segments of $K\beta$ and $K\alpha_{12}$ parts were fitted by the “local” (spreading over the range of 5 pixels to the left and 5 pixels to the right from the local intensity maximas) Gaussian function from which the centre and the width of the peaks were determined and plotted as a function of D .

Figure S1a shows X/D intensity map (summed along Y as in Figure S1b). The numbers on the top describe the reconstructed angular deviation (in mrad) of the beam direction from the normal to the detector plane. This shows that the angle between $K\beta$ and $K\alpha_{12}$ beam centres is 3.83 mrad. This angle is high enough to eliminate all the remainders of $K\beta$ line by a pinhole of 1 mm in diameter. This means that even without a monochromator, we can obtain a parallel beam, suitable for those applications where the separation of $K\alpha_{12}$ duplet is irrelevant (e.g. when e.g. $K\alpha_2$ line can be removed by the data processing). The effective divergence of the $K\alpha_{12}$ doublet part of the beam appears to be <0.2 mrad (this data is further refined later in the paper by measuring the width of diffraction peaks from silicon single crystal). The similarly organized Y/D intensity map in Figure S1b demonstrates that the vertical divergence is also less than <0.2 mrad.

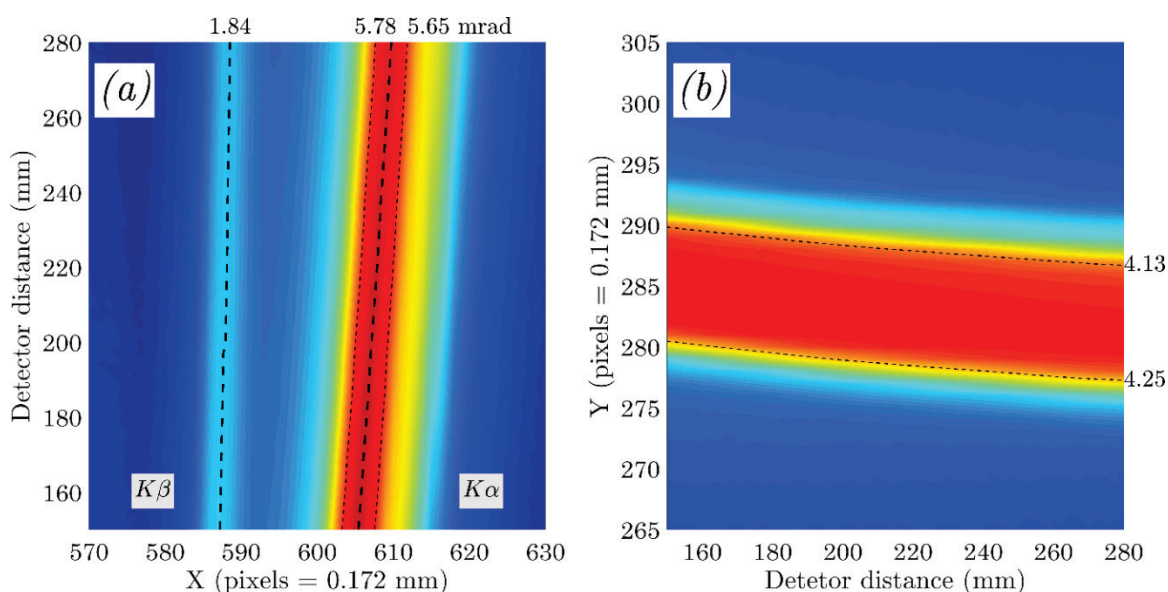


Figure S1 The parameters of the primary X-ray beam, determined by “photographing” the beam at different detector distances. (a) X/D intensity map (summed along Y). (b) Y/D intensity map (summed along X). The numbers on the top and on the right of the graphs indicate the angular deviation of the beam in the horizontal and vertical plane (in mrad).