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Use of 2D X-ray Detector in Powder Diffraction Measurement

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Introduction

We can now use 2D X-ray detectors.

Question 1:

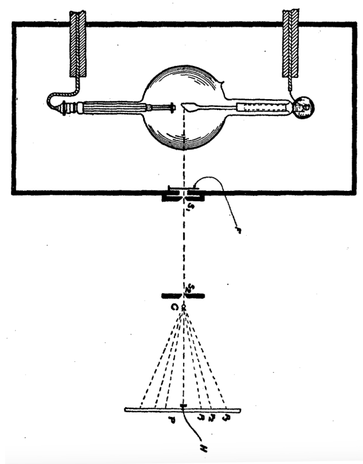
Are 2D data useful for powder diffraction ?

Question 2:

How should the 2D powder instrument be designed ?

Question 3:

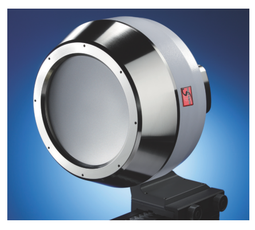
How can we treat 2D powder diffraction data ?



Hull [1]
Photograph

Dectris
PILATUS 100K
(172 μm pixel)

Rigaku
HyPix-3000
(100 μm pixel)



BrukerAXS
VÅNTEC-500
(68 μm pixel)

PANalytical
PIXcel
(55 μm pixel)

Fig. 1 2D X-ray detectors

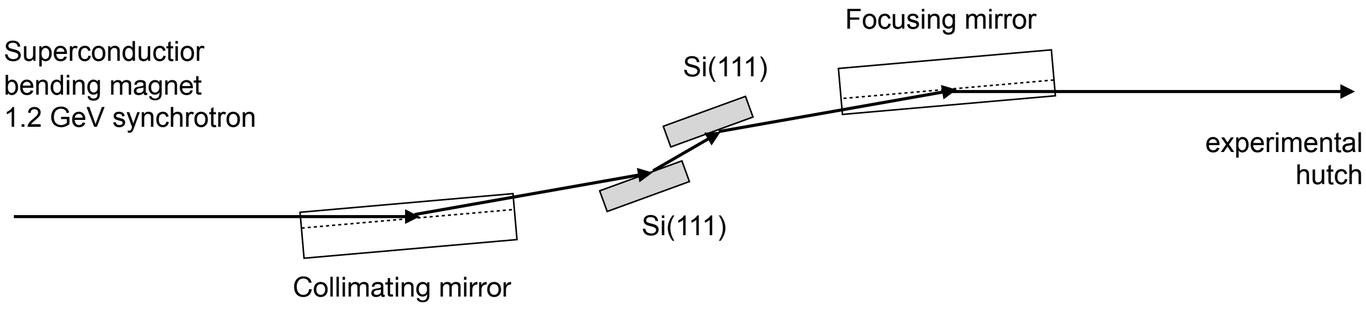


Fig. 2 Schematic configuration of AichiSR BL5S2 beam line optics

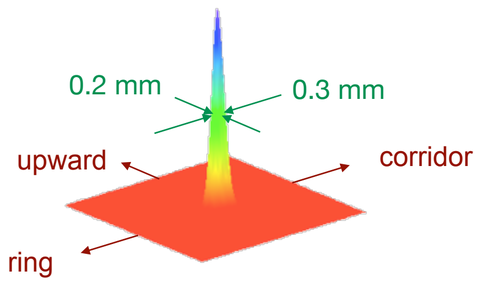


Fig. 3 Cross-section intensity distribution of the AichiSR BL5S2 incident beam, recorded with an Imaging Plate

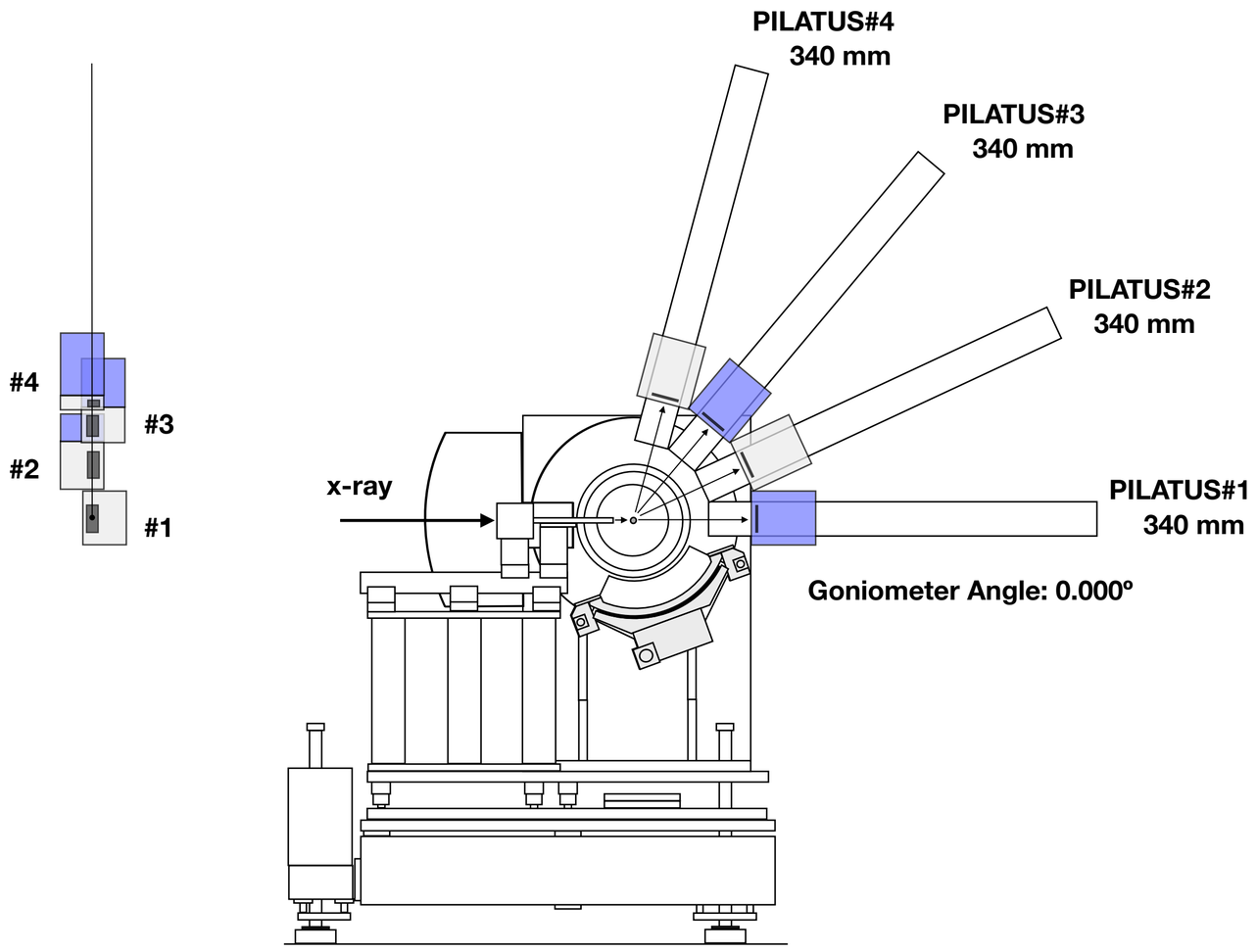
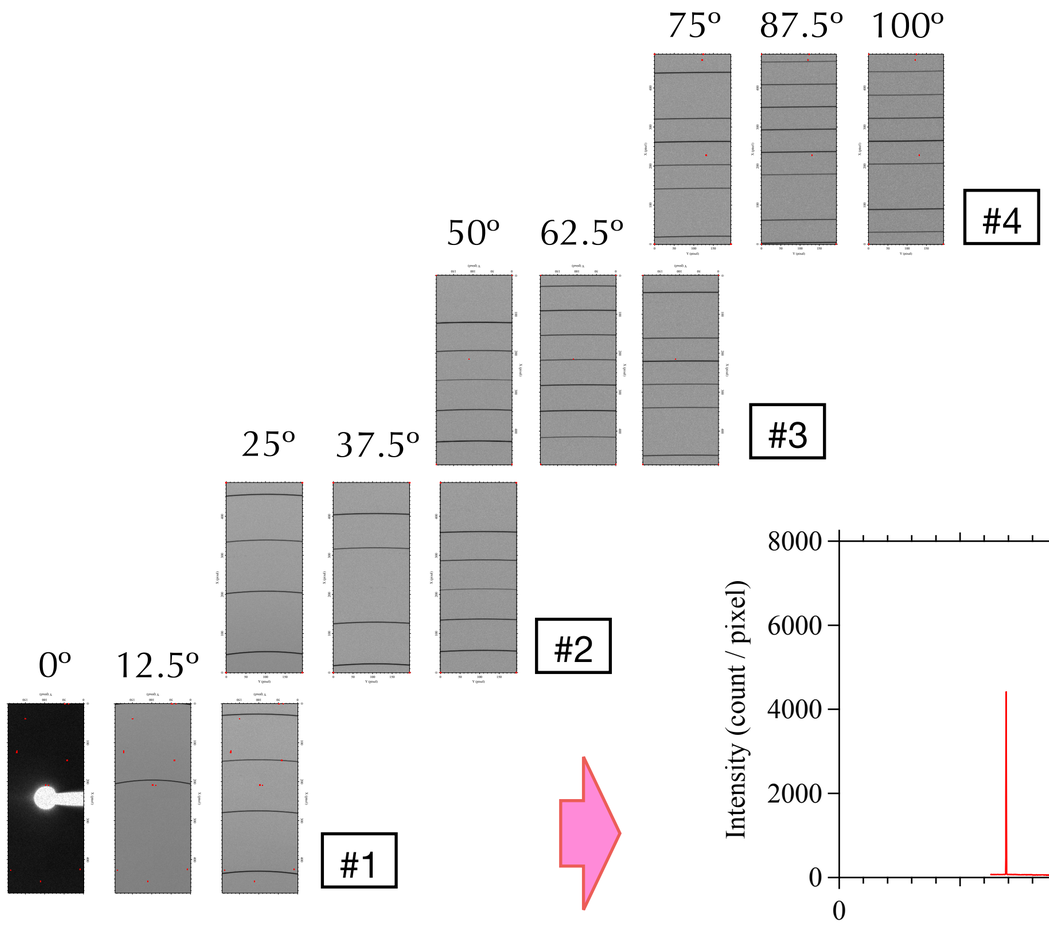
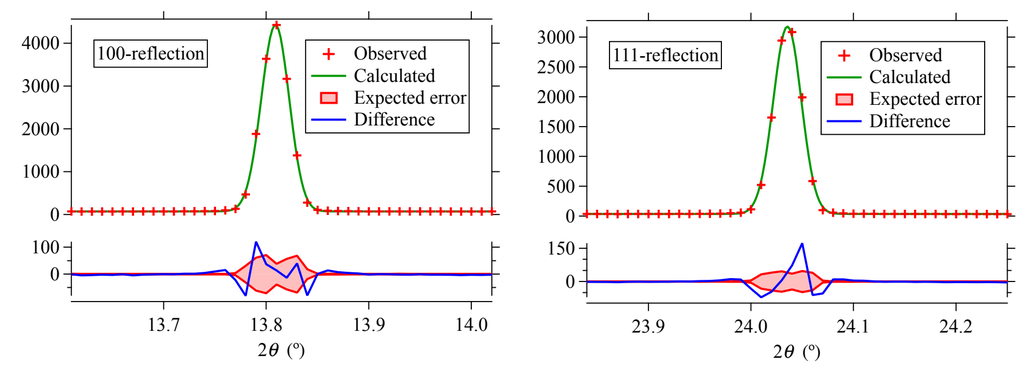


Fig. 4 Straight formation of 4-Pilatus detectors on the AichiSR BL5S2 beam line. Camera length : 340 mm – 1000 mm





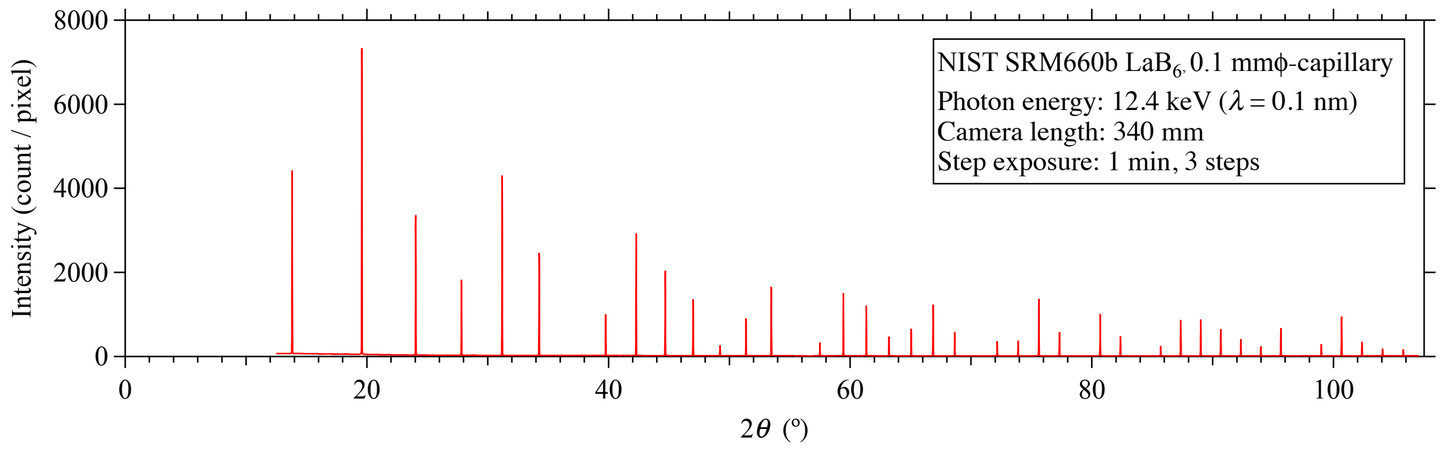
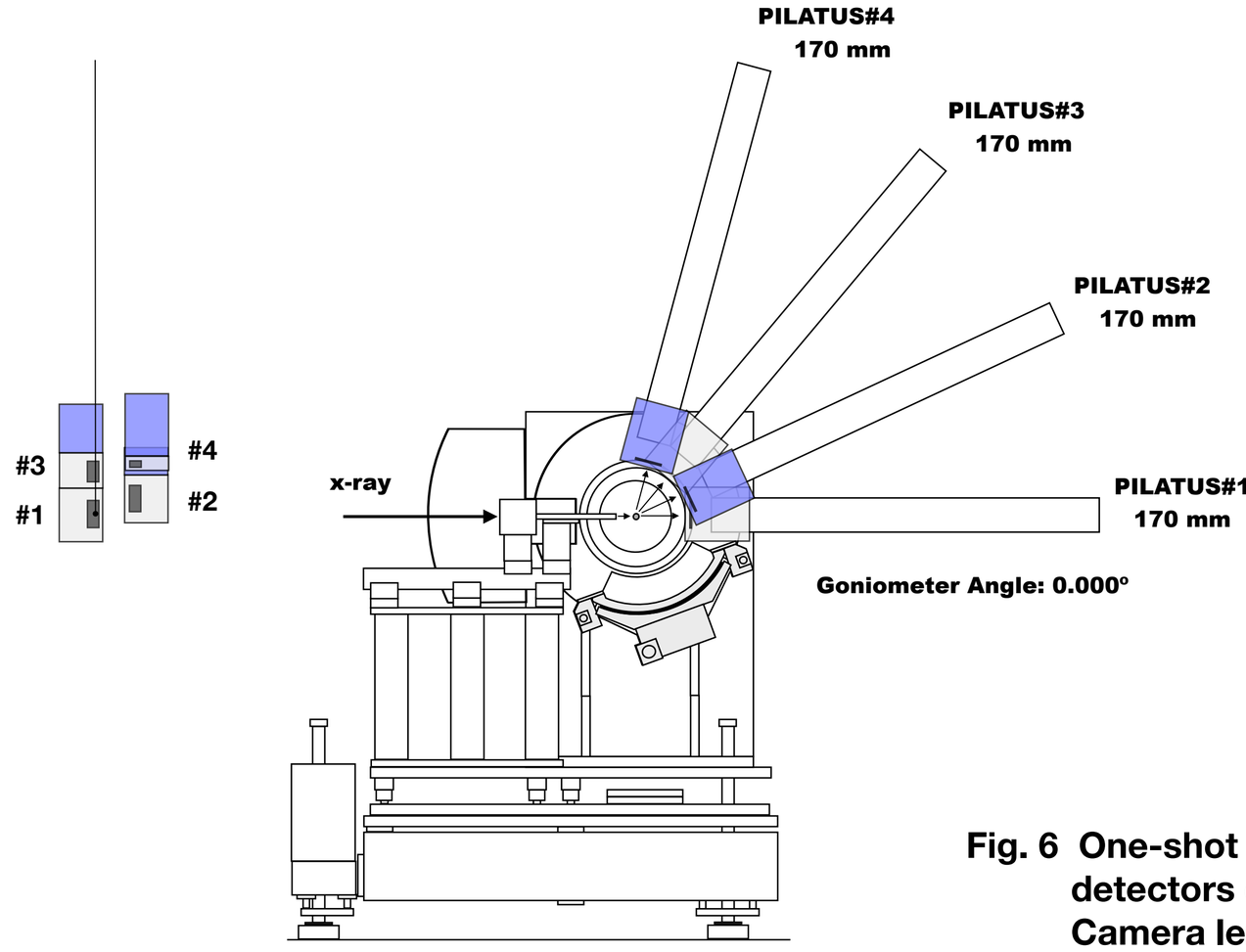


Fig. 5 NIST SRM660b LaB_6 profile synthesized by 3-shot (1 min / each) data of 4 Pilatus detectors on the AichiSR BL5S2 beam line.



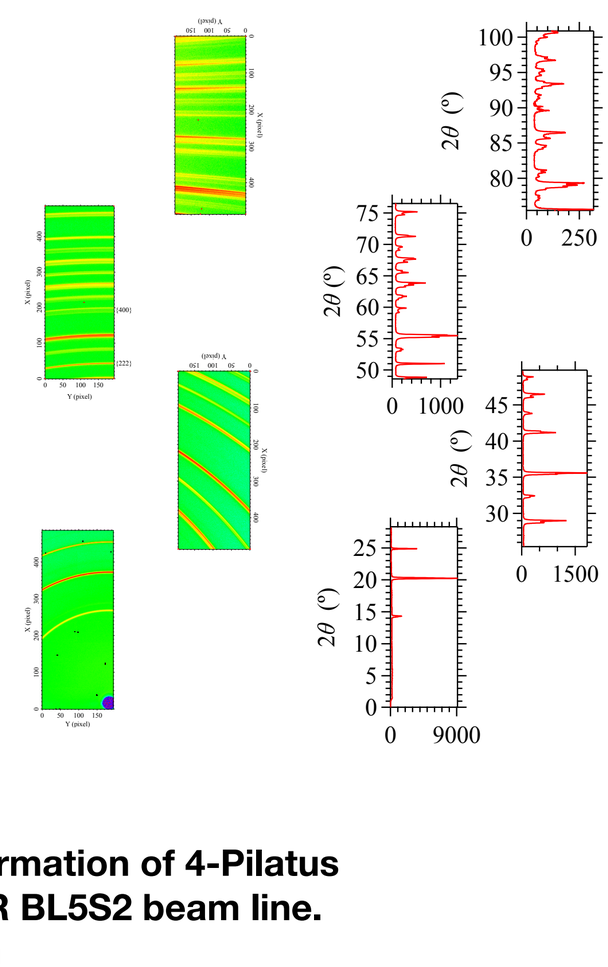


Fig. 6 One-shot (off-center) formation of 4-Pilatus detectors on the AichiSR BL5S2 beam line. Camera length : 170 mm

Advantages of flat 2D detectors

(1) Rapid measurement

– Getting more pronounced

(2) Free of aberration

– Integration along Debye-Scherrer or Hull rings.
– Combination with convergent synchrotron beam is particularly effective.

(3) Error estimation available

– Statistical errors can be evaluated by experiment [2].
– Maximum likelihood estimation can be achieved just by weighted least-squares method.

Disadvantages of flat 2D detectors

(1) Higher cost

– Getting more reasonable

(2) Lower angular resolution

– Getting improved.

(3) Higher background

– Probably unavoidable
– Reducible by elimination of stray-light or use of evacuated or He-filled path ?

(4) Mapping to 1D data required

– Automatic method has already been proposed [2,3].

(5) Difficulty in adjustment and/or calibration

– Calibration method is under development.

References

[1] A. W. Hull, *Phys. Rev.* **10**, 661–697 (1917). [2] T. Ida, *Powder Diffr.* (submitted). [3] S. N. Sulyanov, A. N. Popov & D. M. Kheiker, *J. Appl. Cryst.* **27**, 934–942 (1994).