



# HARDWARE SETTINGS OF X-RAY POWDER DIFFRACTION

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# THE OPTICAL ELEMENTS OF XRD INSTRUMENT

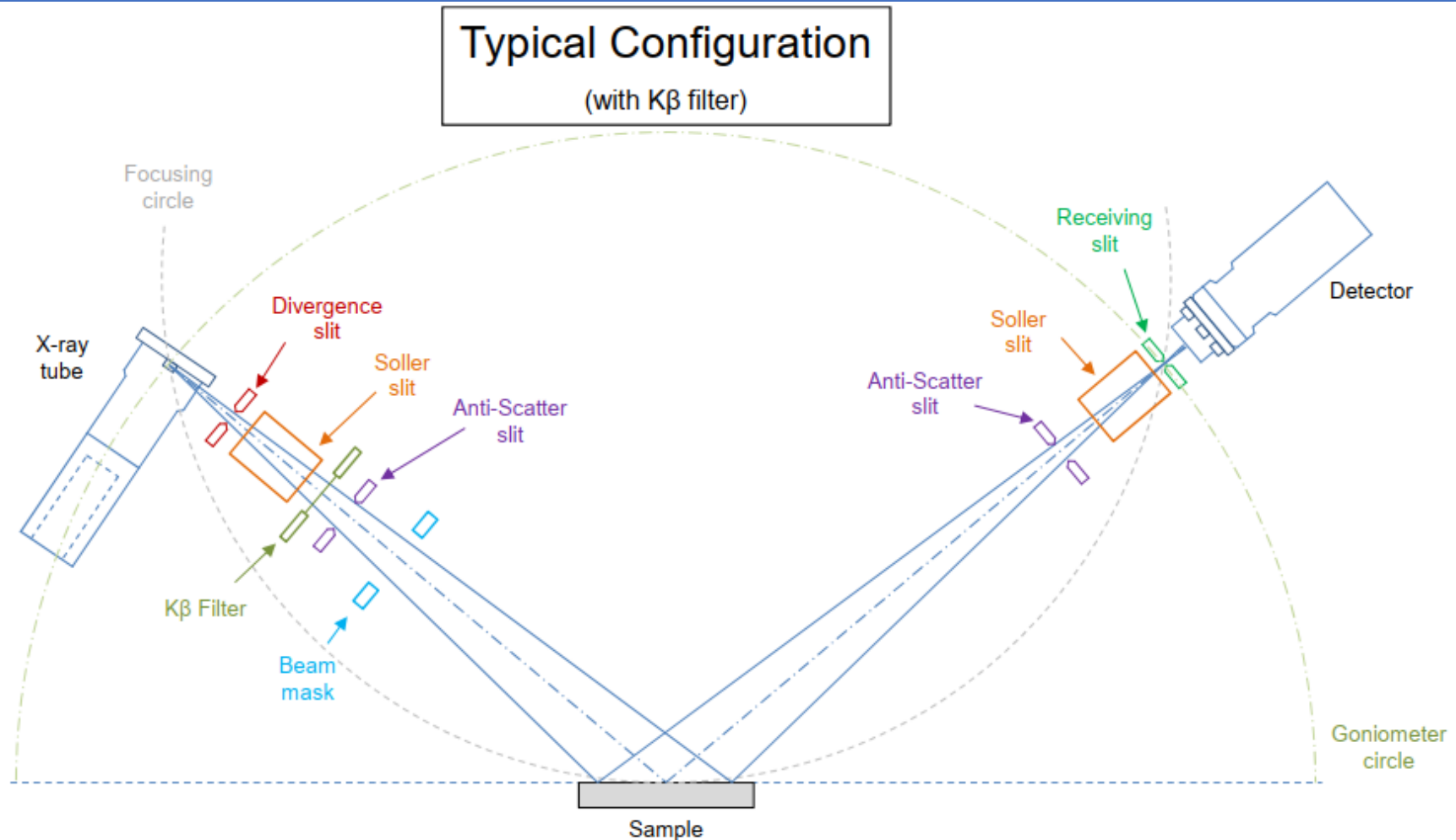
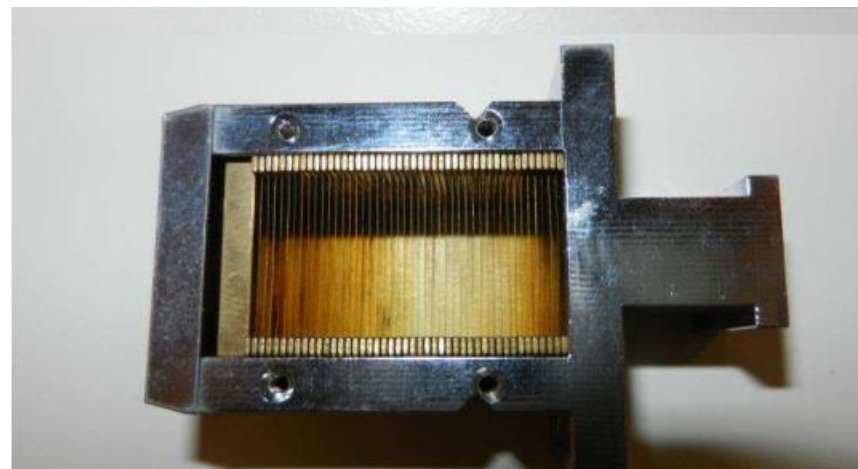


Figure source: Nicola, Döbelin, lesson 2 Diffractometers and phase identification, RMS foundation, Switzerland

# SOLLER SLIT

- Soller slit consists of large numbers of parallel metal plates in plane of diffraction
- It can limit the axial divergence of incident & diffracted X-ray beam and reduces peak asymmetry
- Using soller slit improves peak shape and resolution, especially at the low scattering angles



# DIVERGENT SLIT

- It is essential to select the appropriate divergent slit to avoid X-ray beam spill-over at low  $2\theta$  angles.
- Refer to the divergent slit chart in the XRD operation manual

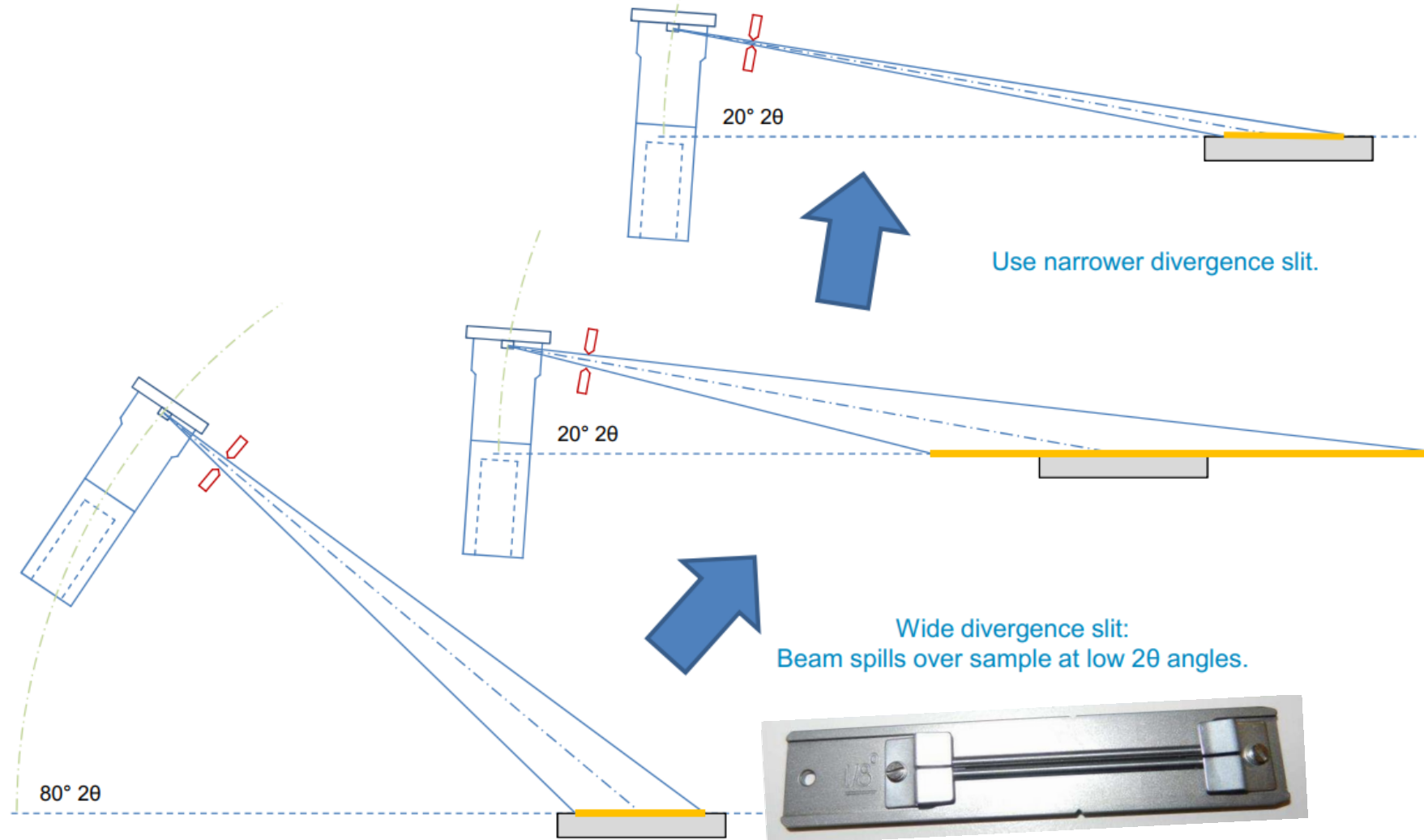
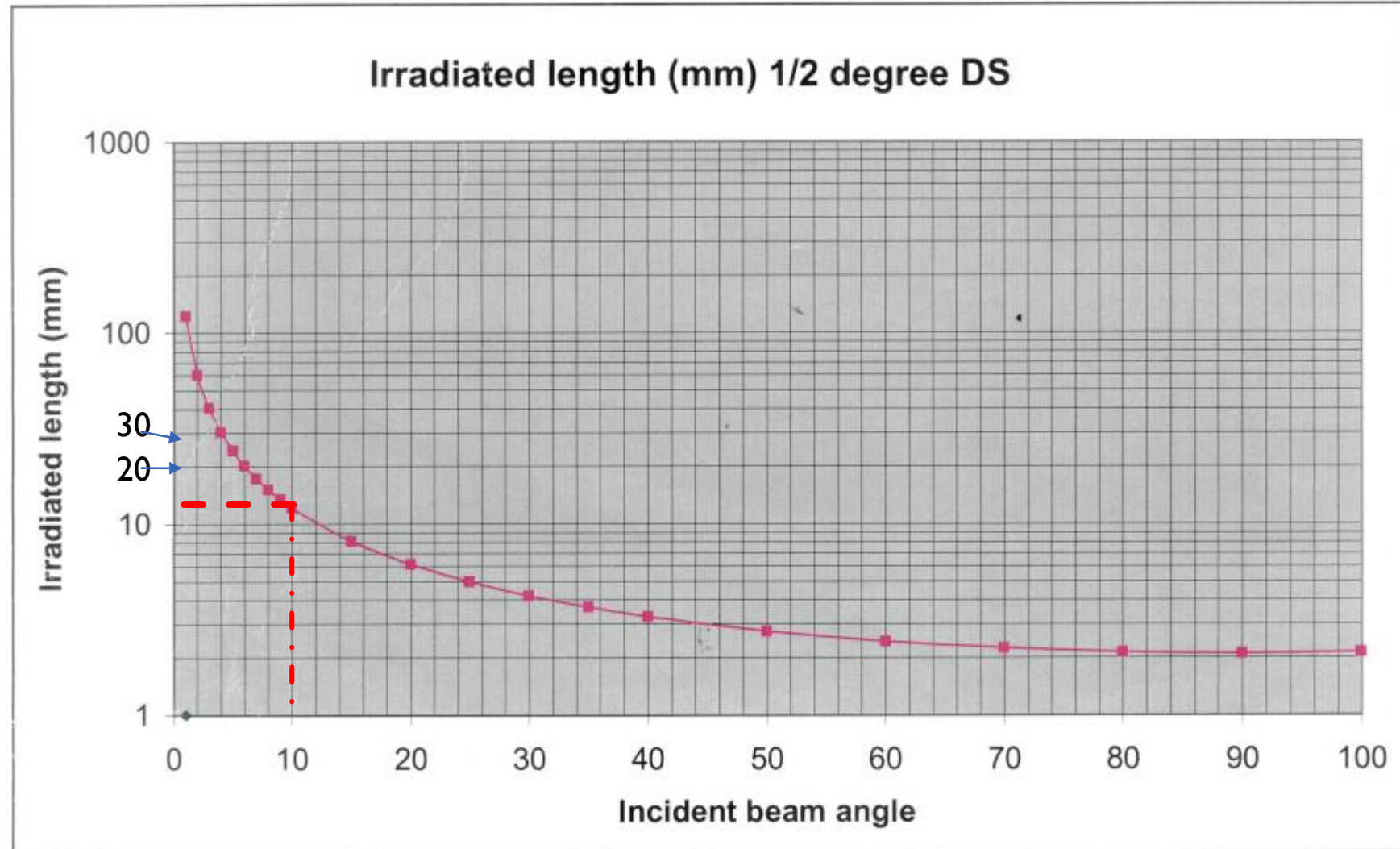


Figure source: Nicola, Dobelin, Lesson 2 Diffractometers and phase identification, RMS foundation, Switzerland

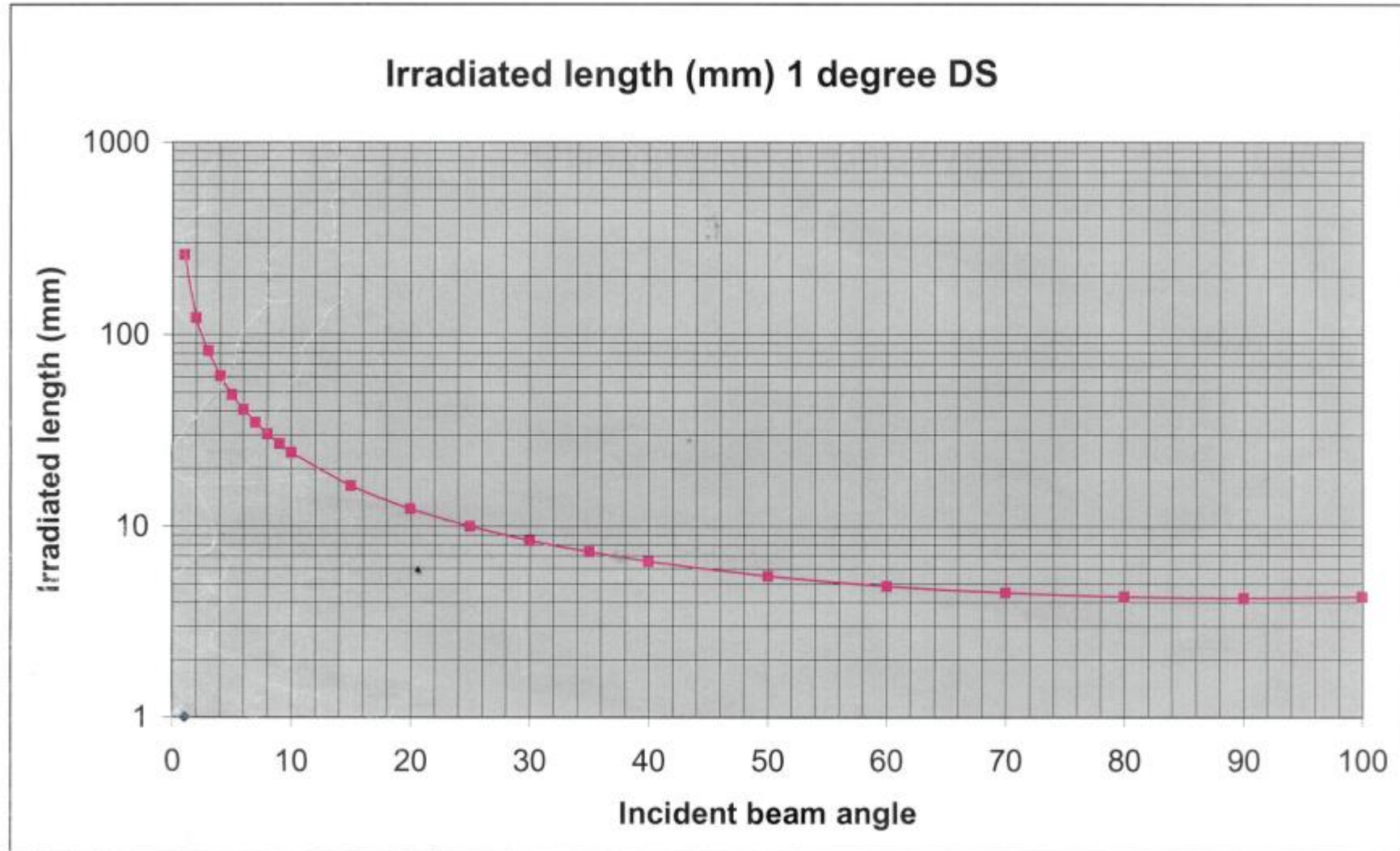
# DIVERGENT SLIT CHART I



For instance,

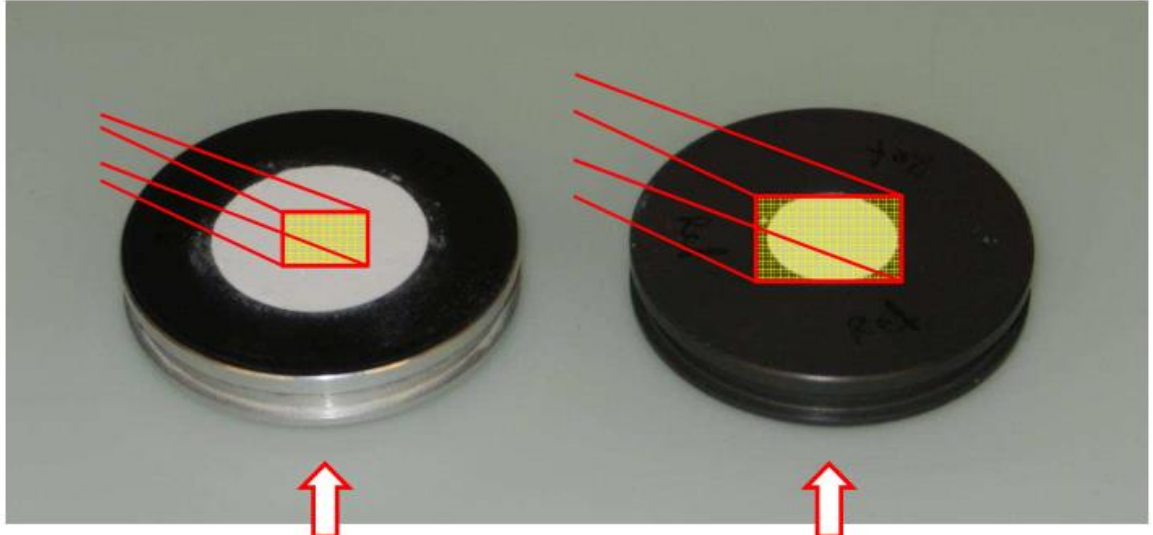
When the divergent slit of  $\frac{1}{2}$  degree is selected, the irradiated length of sample is between 10 and 20 mm.

# DIVERGENT SLIT CHART 2



➔ Match your Divergence Slit and Beam Mask!

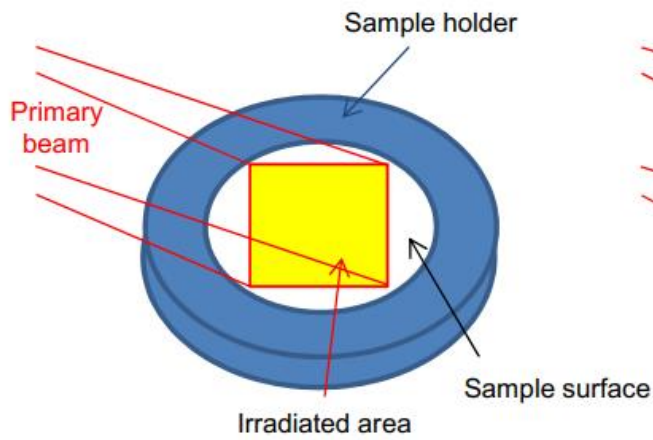
# MASK



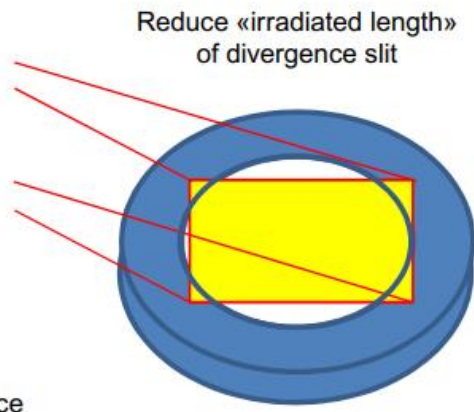
Or else: Waste of intensity or Beam spill-over

Since the X-ray beam is broadening from X-ray tube to sample stage, it is recommended to use the mask, where the width of mask is smaller than that of the sample width.

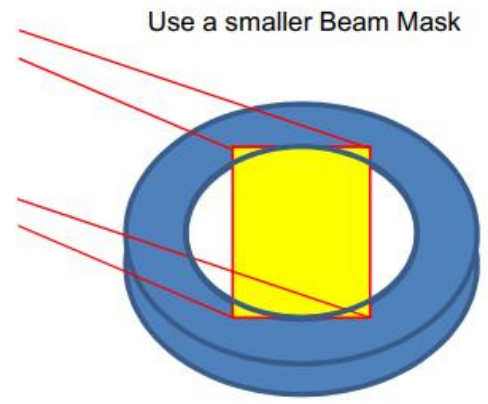
Correct!



Wrong!



Wrong!



# RECOMMENDED MEASUREMENT PARAMETERS

Optical elements	Functions and recommended settings
Beta filter	Generally applied to remove $K_{\beta}$ characteristic lines
Soller slit	Generally applied to correct the axial divergence of both incident & diffracted beams 0.04 radians for general scan, and 0.02 radians for high-resolution scan
Beam mask	For <b>MPD or Empyrean II</b> instrument For 30mm sample holder, 15 mm mask is recommended For 15mm sample holder, 10 mm mask is recommended
Divergent slit	For <b>MPD or Empyrean II</b> instrument (start angle > 10 degree) For 30mm sample holder, 1 degree divergent slit is recommended For 15mm sample holder, 1/2 degree divergent slit is recommended