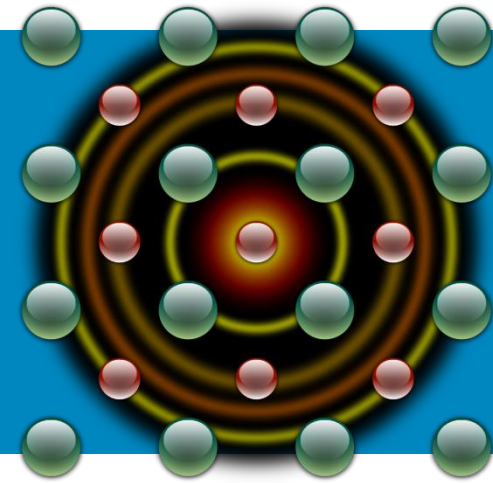


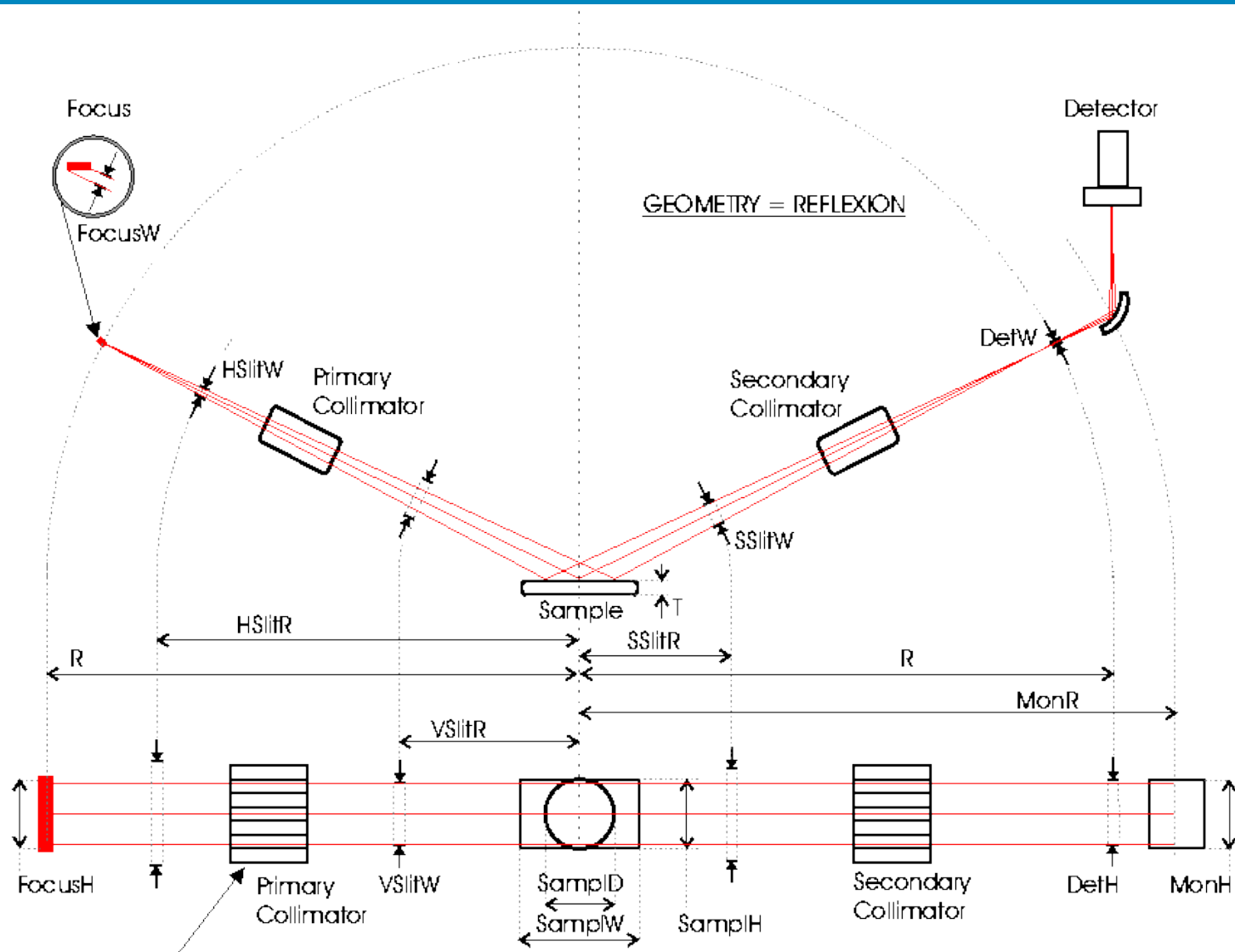
# Lesson 3

## Example Instrument Configuration



Nicola Döbelin  
RMS Foundation, Bettlach, Switzerland

# Fundamental Parameters Approach



<http://www.bgm.de>

# BGMN Instrument Configuration Files (\*.sav)

```
%*****  
%  
%   BGMN Device Configuration File for Bruker D8  
%   -----  
%  
%   Created by Nicola Doebelin, RMS Foundation, CH  
%   December 11, 2014  
%  
%   Device Configuration:  
%   - Detector: LynxEye XE  
%   - Radiation: CuK $\alpha$   
%   - Soller Slits: 2.5°  
%   - Divergence Slit: Automatic 15mm  
%   - Anti-Scatter Slit: 9mm  
%   - Goniometer Radius: 350 mm  
%  
%*****  
%-----  
% Output files for Geomet and MakeGeq  
%-----  
  
VERZERR=RMS-D8-ADS-15-LynxEyeXE.ger  
GEQ=RMS-D8-ADS-15-LynxEyeXE.geq
```

Comment header

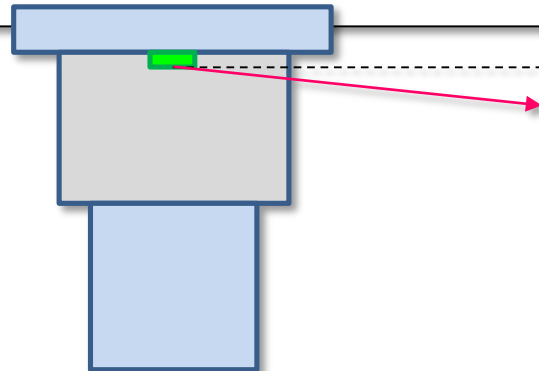
'%' = comment character

Names of output files: basename  
**must** be identical to this  
configuration file.

(Change if configuration file is  
saved under a new name)

# BGMN Instrument Configuration Files (\*.sav)

```
%-----  
% Goniometer geometry  
%-----  
  
% REFLEXION = Bragg-Brentano parafocusing  
GEOMETRY=REFLEXION  
  
% Goniometer radius (mm)  
R=350  
  
%-----  
% X-ray tube  
%-----  
  
% axial dimension (length, mm)  
FocusH=12  
  
% optical breadth (1/10 of nominal) of the line focus (mm)  
FocusW=0.04
```



Apparent size of the tube target

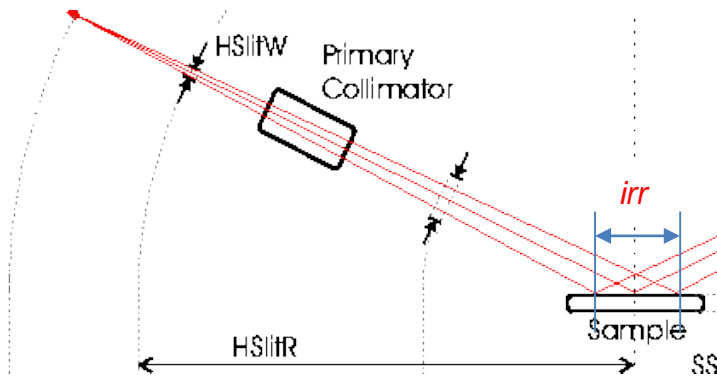
Typical real target size: 12 x 0.4 mm

«Take-off Angle»: 6°

Apparent size:  $0.4 \text{ mm} * \sin(6^\circ) = 0.04 \text{ mm}$

# BGMN Instrument Configuration Files (\*.sav)

```
%-----  
% Divergence slit  
%-----  
  
% irradiated length (mm)  
irr=15  
  
% distance from sample (mm)  
HSlitR=250  
  
% automatic divergence slit width (mm)  
HSlitW=(2*(R-HSlitR)*irr*sin(pi*zweiTheta/360))/(2*R+irr*cos(pi*zweiTheta/360))
```



Distance *HSlitR* and width *HSlitW* are used to calculate irradiated length *irr* on the sample surface

In Automatic Divergence Slit (ADS) mode *HSlitW* is variable.

*irr* is not a BGMN variable, just a custom helper variable

*HSlitW* can be calculated from *irr*, *R*, *HSlitR*, and as a function of *zweiTheta* ( $2\theta$ ).

# BGMN Instrument Configuration Files (\*.sav)

```
%-----  
% Detector  
%-----  
  
% total detector height (mm)  
DetArrayW=14.4  
  
% height of one strip (mm)  
DetW=0.075  
  
% total detector width (mm)  
DetH=16
```

Specifications for LynxEye XE detector:

Width = 16 mm

192 pixel strips of 75  $\mu\text{m}$  height  
→ Height = 14.4 mm

User Manual

LYNXEYE XE Detector

## 4.1 The Detector

### 4.1.1 Detector Specifications

Table 4.1: Basic specifications of the LYNXEYE XE

Detector Specifications	
Suitable systems	All D8 diffraction solutions systems with DIFFRAC.Measurement Suite V3 or higher.
Active area	14.4 mm (192 x 0.075mm) x 16 mm; (in and perpendicular to the scattering plane)
Max 2-theta range simultaneously covered	3,3° at 500 mm measurement circle diameter
Usable wavelength range	Cr, Co, Cu, Mo, and Ag radiation. Factory settings are optimized for Cu-K $\alpha$

# BGMN Instrument Configuration Files (\*.sav)

```
%-----  
% Sample holder  
%-----  
  
% diameter of the sample holder (mm)  
SamplD=25  
  
%-----  
% Collimators (Soller slits)  
%-----  
  
% Note: For some manufacturers we have to use half the  
% opening angle given on the soller slits (Bruker), but  
% for others (Panalytical) we have to use the full value.  
% Here soller slits of 2.5° were used, which is 0.0436  
% radians. We use 0.0436 / 2 = 0.0218 rad.  
  
% primary soller slit (radians)  
PColl=0.0218  
  
% secondary soller slit (radians)  
SColl=0.0218
```

# BGMN Instrument Configuration Files (\*.sav)

```
%-----  
% Beam Mask / Primary Beam Anti-Scatter Slit  
%-----  
  
% Beam width (mm)  
VSlitH=20.0  
  
% distance from sample (mm)  
VSlitR=200  
  
%-----  
% Beam Knife  
%-----  
  
% AirScat=3.5  
  
%-----  
% Secondary Beam Anti-Scatter Slit  
%-----  
  
% distance from sample (mm)  
SSlitR=180  
  
% slit width (mm)  
SSlitW=9
```

Empty slit mount has a width  
of 20 mm

No beam knife installed,  
disabled (note comment sign '%')

Installed, but not in use,  
always wide open (9 mm)



# BGMN Instrument Configuration Files (\*.sav)

```
%-----  
% Monochromator  
%-----  
  
% None used  
% MonR=  
% MonH=
```

No monochromator installed,  
disabled (note comment sign '%')

# BGMN Instrument Configuration Files (\*.sav)

```
%-----  
% Parameters for the simulation of the profile function  
%-----  
  
% angular positions for the MonteCarlo simulation (°2theta)  
zweiTheta[1]=4  
zweiTheta[2]=8  
zweiTheta[3]=13  
zweiTheta[4]=20  
zweiTheta[5]=30  
zweiTheta[6]=42  
zweiTheta[7]=56  
zweiTheta[8]=76  
zweiTheta[9]=90  
zweiTheta[10]=105  
zweiTheta[11]=120  
zweiTheta[12]=135  
zweiTheta[13]=150  
  
% angular range for profile interpolation (°2theta)  
WMIN=4  
WMAX=150  
  
% step width for profile interpolation (°2theta)  
WSTEP=2*sin(pi*zweiTheta/180)
```

2θ angles for peak profile  
raytracing

Must cover the entire range  
of future measurements

Range and stepsize of peak  
profile interpolation

Set WMIN and WMAX to the  
same range as zweiTheta above

Leave WSTEP unchanged

# BGMN Instrument Configuration Files (\*.sav)

```
% switch for applying the intensity correction for beam
% overflow resp. ADS function
GSUM=Y

% Use multithreaded calculation
NTHREADS=8

% Convenience function: Calculate PI for use in other
% angle-dependent calculations
pi=2*acos(0)

% Do not alter the SAV file
SAVE=N

%-----
% End of file
%-----
```

Leave all variables  
unchanged

NTHREADS > 1 does not  
work in BGMN 4.2

- Exercise 1: Configure the RMS standard instrument setup, starting from a totally wrong template.
- Exercise 2: Configure an instrument with a primary beam monochromator.  
(Nobody has succeeded yet...)