**Type of experiment**: XRD

**Author(s)**: Jakub Nowak, Philipp Keuter

**Comments:**

Combined metadata template for the XRD for B02 and C03

------------------------------------------------------------------------------------------------------------

*PLEASE DO NOT CHANGE THIS – USE COMENTS TO INCUDE MORE INFO!*

**Legend:**

**Bold** shows the metadata to be included

(brackets) show what type of value is associated, e.g. ‘string’ *“this is a string”*, int *5*, float *3.33*, or fixed set of options *[“red”, “blue”, “green”]*.

*Italic* font shows the example user input

Light blue highlights meta data to be included in a CoScInE mask for new ressources

Light green highlights meta data that is important but is preserved in other files for now and could later be captured automatically (please still include here explicitly!)

Light yellow highlights meta data that may be inserted as part of another experiment (here = “metallographic preparation” or might be better to keep with the imaging records – t.b.d.

Light grey that this meta data is not essential but might be good include (please do include here whatever meta data you can think of for now!

Please define all but the most trivial of acronyms!

You can provide structure to your metadata by including a **[descriptive header]** and then including sub-pieces of metadata tab-indented.

------------------------------------------------------------------------------------------------------------

**Operator** (string)

*Your Name*

**Experiment ID** (string)

*e\_77\_xyz*

**Instrument used** (string)

*GADDS\_MCh*

**Measurement date/time** (string)

*10.04.2020*

**Specimen Type (“Thin Film”, “Bulk”)**

*Thin Film*

**[Parameter if Specimen Type “Thin Film” is chosen]**

**Specimen ID** (string)

*e\_77*

**[Parameter if Specimen Type “Thin Film” is chosen]**

**Parent sample specimen ID** (string, or maybe drop down of existing data)

*S3\_Mg-Ca\_P19*

**Preparation routine** (string, or maybe drop down of existing data)

*Metallo\_03*

**Pre-treatment** *(“grinding”, “polishing”, “immersion”)*

Polishing

**Sample storage** (“air”, “dissicator”, “high vacuum”, “protective gas – Ar”,”…”) (single choice)

*Dissicator*

**Immersion Experiment ID** (string, or maybe drop down of existing data)

xyz\_11.11.2020

**Radiation source** (Options: “Cu”, “Co”)

*Cu*

**Detector** (“point”, “Line”, “2D”, “open”)

point

**Current [mA]** *(integer)*

*40*

**Voltage [kV]** *(integer)*

*40*

**[This is per aquisition]**

**Measurement position** (string)

*5 mm from left edge, 1mm above red marker, P17*

**Scan Mode** (Bragg-Brentano, Detector Scan, unlocked coupled, Rocking curve)

*Detector scan*

**Comments** (string)

*k-alpha2 stripped*

**Filter** *(string)*

*Bruker Metal*

**Mask size** *[mm] (string)*

*25 x 25*

**[Parameter if detector scan is chosen]**

**Scan axis** (options: 2Theta, Chi, Phi)

*2Theta*

**Incidence angle Omega [°]** (float)

*15*

**Diffraction angle 2Theta [°]** (float)

*30*

**Rotation angle phi [°] (float)**

*0*

**Rotation angle chi [°] (float)**

*0*

**Number of frames** (int)

*2*

**Measurement time [s]** (int)

*300*

**[Parameter if Bragg-Brentano, Rocking curve, unlocked coupled scan is chosen]**

**Start 2Theta [°]** (float)

*10*

**End Theta [°]** (float)

*85*

**Start Theta [°]** (float)

*5*

**Fixed 2Theta position [°]** (float)

*5*

**Step size [°]** (float)

*0.02*

**Time per step [s]** (float)

*3*