the file formats working group

presents a draft for a

simple model language

by

Jochen Stahn Paul Scherrer Institut, Switzerland

Artur Glavic Paul Scherrer Institut, Switzerland

Brian Maranville NIST, USA

simple model language

aims

experiment planning

estimate counting times and statistics

plan and experimental settings

completeness of reflectivity file

sample names are non-descriptive

a sample model in the `.ort` file is useful
for everyone not in posession of the log book(s)

data analysis

allow analysis software to automatically
create a starting model

indexing of data

used for indexing, searchning and filing

e.g. to train AI algorithms

simple model language

concept

intuitive and simple to start

→ `air | 5 ( Fe 6 | Ti 7 ) | Si`

standardised

the beam enters from the left

`stack` and `sub_stacks` are strings

details are organised following a YAML structure

expandable

magnetic layers

sub-structures

definition of sub-stacks, layers, compositions and materials

refering to external databases

ORSO SLD Database, own definitions, . . .

compatibility

seamless integration into `.ort` specifications

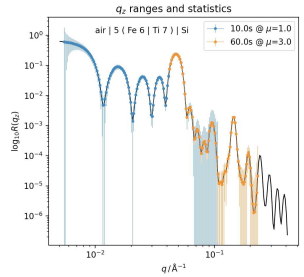
simple model language

use case

sample declaration in instrument software

```
air | 5 ( Fe 6 | Ti 7 ) | Si
```

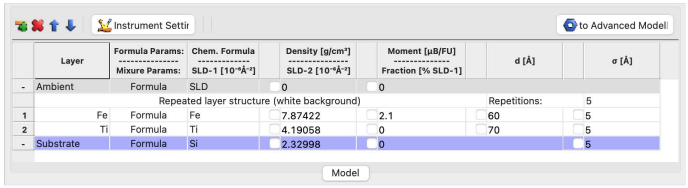
quick & dirty simulation of $I(q_z)$ for **experiment planning**



hand-over to raw and reduced **data file** (`.ort`)

```
#  model:
#    origin:  NICOS input mask
#    stack:  air | 5 ( Fe 6 | Ti 7 ) | Si
#    globals:
#      length_unit:  nm
```

used by **analysis software** to generate initial fitting model



simple model language

sample declaration

sample declaration

name: [ ]

type: [▼ please choose]

size: [ ] × [ ] mm^2

description: [ ]

---

model: [ ]

☐ expand

☐ simulate

α_i / deg	1.0	2.0	–	–
t / s	10	60	–	–
spin	o	o	o	o

simple model language

sample declaration

sample declaration

name: JS_2021_09_21_1

type: ▼ solid film on substrate

size: 10 × 10 mm^2

description:

---

model: air | 5 (Fe 6 | Ti 7) | Si

☐ expand

☐ simulate

α_i / deg	1.0	2.0	–	–
t / s	10	60	–	–
spin	o	o	o	o

An iron - titanium multilayer on silicon
with 5 repetitions and
layer thicknesses of 6 nm and 7 nm, respectively.

simple model language

sample declaration

model: `air | 5 ( Fe 6 | Ti 7 ) | Si`

☐ expand

☐ simulate

α_i/ deg	1.0	2.0	–	–
t/ s	10	60	–	–
spin	o	o	o	o

simple model language

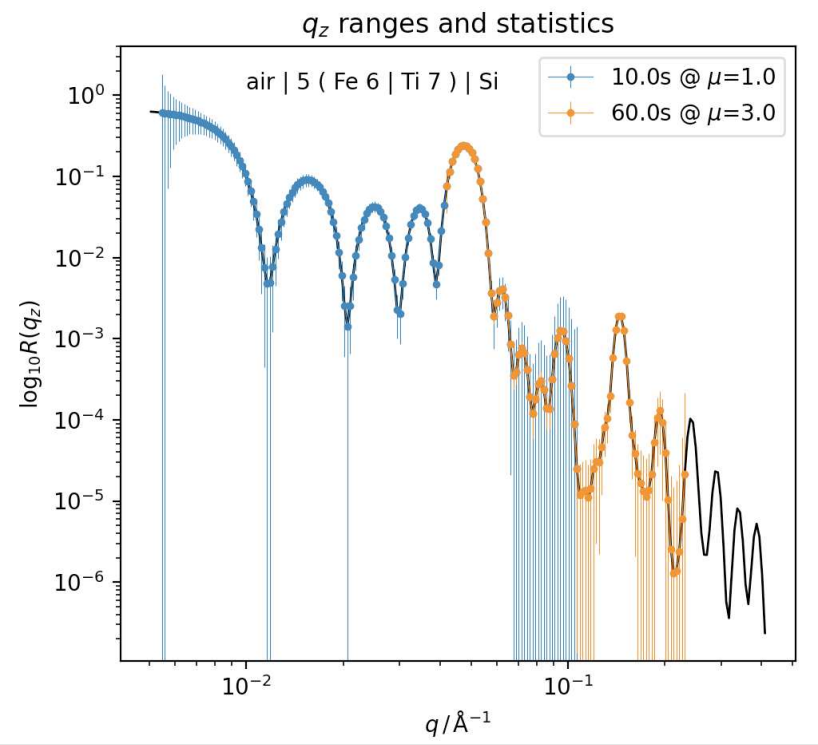
sample declaration & experiment planning

model: `air | 5 ( Fe 6 | Ti 7 ) | Si`

☐ expand

☒ simulate

α_i/ deg	1.0	3.0	–	–
t/ s	10	60	–	–
spin	o	o	o	o



simple model language

sample declaration & experiment planning

model: `air | 5 ( Fe 6 | Ti 7 ) | Si`

☒ expand

layer	formula	SLD*	ρmass	M/μ_B	ρrel
air		0.0	0.0	0.0	1.0
Fe	Fe	7.6	7.874	0.0	1.0
Ti	Ti	-3.2	4.54	0.0	1.0
Si	Si	2.22	2.33	0.0	1.0

☐ simulate

α_i/ deg	1.0	3.0	–	–
t/ s	10	60	–	–
spin	o	o	o	o

simple model language

sample declaration & experiment planning

model: `air | 5 ( Fe 6 | Ti 7 ) | Si`

☒ expand

layer	formula	SLD*	ρmass	M/μ_B	ρrel
air		0.0	0.0	0.0	1.0
Fe	Fe	7.6	7.874	2.1	1.0
Ti	Ti	-3.2	4.54	0.0	0.93
Si	Si	2.22	2.33	0.0	1.0

☐ simulate

α_i/ deg	1.0	1.0	3.6	3.6
t/ s	10	10	80	80
spin	p	m	p	m

simple model language

sample declaration & experiment planning

model: `Si | my_lipid 2 | toluene`

☒ expand

layer	formula	SLD*	ρmass	M/μ_B	ρrel
Si	Si	2.22	2.33	0.0	1.0
my_lipid				0.0	1.0
toluene				0.0	1.0

☐ simulate

α_i/ deg	1.0	2.0	–	–
t/ s	10	60	–	–
spin	o	o	o	o

simple model language

sample declaration & experiment planning

model: `Si | my_lipid 2 | toluene`

☒ expand

layer	formula	SLD*	ρmass	M/μ_B	ρrel
Si	Si	2.22	2.33	0.0	1.0
my_lipid		1.3		0.0	1.0
toluene	C7H8		0.83	0.0	1.0

☐ simulate

α_i/ deg	1.0	2.0	–	–
t/ s	10	60	–	–
spin	o	o	o	o

simple model language

syntax

so far we have used

model: `air|5 (Fe 6|Ti 7)|Si`

expansions: magnetic moment
relative density
formula
mass density

simple model language

syntax

so far we have used

model: `air|5 (Fe 6|Ti 7)|Si`

expansions: magnetic moment
relative density

formula
mass density

and this is the expression
in the model language:

```
model:
  origin:  NICOS input mask
  stack:  air | 5 ( Fe 6 | Ti 7 ) | Si
  materials:
    Fe:  {magnetic_moment:  2.1}
    Ti:  {rel_density:  0.93}


    toluene:
      formula:  C7H8
      mass_density:  0.83
    my_lipid:  {SLD: 1.3}

  globals:
    length_unit:  nm
    SLD_unit:  1E-6/angstrom^2
    mass_density_unit:  g/cm^3
    magnetic_monent_unit:  muB
```

simple model language and the .ort file

sample declaration

name: JS_2021_09_21_1

type: ▼ solid film on substrate

size: 10 × 10 mm^2

description:

---

model: air | 5 (Fe 6 | Ti 7) | Si

☐ expand

```
#    sample:
#        name:  JS_2021_09_21_1
#        type:  solid film on substrate
#        model:
#            origin:  NICOS input mask
#            stack:  air | 5 ( Fe 6 | Ti 7 ) | Si
#            globals:  {length_unit:  nm}
```

simple model language and the .ort file

model: `air | 5 ( Fe 6 | Ti 7 ) | Si`

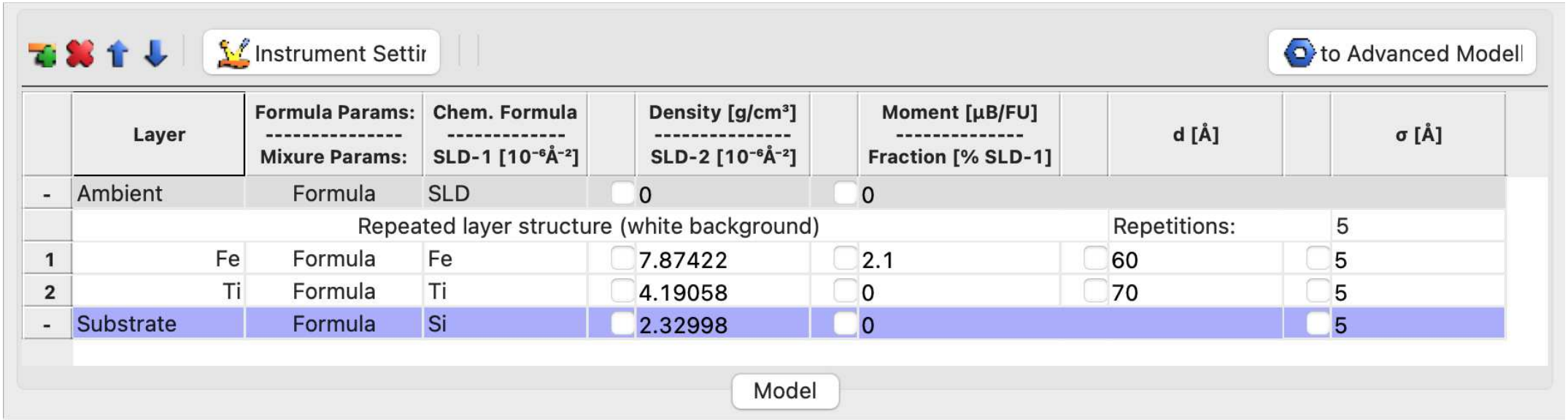
☒ expand

layer	formula	SLD*	ρmass	M/μ_B	ρrel
air		0.0	0.0	0.0	1.0
Fe	Fe	7.6	7.874	2.1	1.0
Ti	Ti	-3.2	4.54	0.0	0.93
Si	Si	2.22	2.33	0.0	1.0

```
#         model:
#             origin:  NICOS input mask
#             stack:  air | 5 ( Fe 6 | Ti 7 ) | Si
#             materials:
#                 Fe:  {magnetic_moment:  2.1}
#                 Ti:  {rel_density:  0.93}
#             globals:
#                 length_unit:  nm
#                 magnetic_monent_unit:  muB
```

simple model language and analysis software

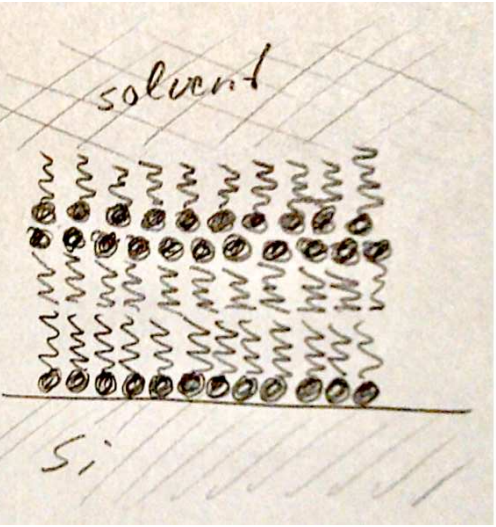
```
#         model:
#             stack:  air | 5 ( Fe 6 | Ti 7 ) | Si
#             materials:
#                 Fe:  {magnetic_moment:  2.1}
#                 Ti:  {rel_density:  0.93}
#             globals:
#                 length_unit:  nm
#                 magnetic_monent_unit:  muB
```



	Layer	Formula Params: / Mixure Params:	Chem. Formula / SLD-1 [10^{-6}Å^{-2}]	Density [g/cm³] / SLD-2 [10^{-6}Å^{-2}]	Moment [μB/FU] / Fraction [% SLD-1]	d [Å]	σ [Å]
-	Ambient	Formula	SLD	0	0		
	Repeated layer structure (white background)					Repetitions:	5
1	Fe	Formula	Fe	7.87422	2.1	60	5
2	Ti	Formula	Ti	4.19058	0	70	5
-	Substrate	Formula	Si	2.32998	0		5

simple model language

more complex constructions




```
#         stack:  Si | LB_ml | solvent
#         sub-stacks:
#             LB_ml:
#                 sequence:
#                  - {material:  head, thickness:  0.5}
#                  - {material:  CH2, thickness:  1.7}
#                  - {material:  CH2, thickness:  1.7}
#                  - {material:  head, thickness:  0.5}
#                  - {material:  head, thickness:  0.5}
#                  - {material:  CH2, thickness:  1.7}
#         composits:
#             solvent:
#                 cyclohexane:  0.4
#                 toluene:  0.6
#         materials:
#             cyclohexane:
#                 formula:  C6H12
#                 mass_density:  0.778
#             toluene:
#                 formula:  C7H8
#                 mass_density:  0.87
#             head:  {SLD: 1.33}
#             CH2:  {mass_density:  0.83}
```

simple model language

borrowing syntax from other model languages

```
#         stack:  Si | LL | rLL | D2O
#         sub_stacks:
#           LL:
#             sequence:
#             - material:  sld:  1.88401254e-06
#               thickness:  9.0
#               roughness:  3.0
#             - material:  sld:  -3.73401535e-07
#               thickness:  1.4
#               roughness:  3.0
#             represents:  refnx.reflect.LipidLeaflet
#             arguments:  [56, 6.01e-4, 319, 9, -2.92e-4, 782, 14, 3, 3]
#           rLL:
#             sequence:
#             - material:  sld:  -3.73401535e-07
#               thickness:  1.4
#               roughness:  0.0
#             - material:  sld:  1.88401254e-06
#               thickness:  9.0
#               roughness:  3.0
#             represents:  refnx.reflect.LipidLeaflet
#             arguments:  [56, 6.01e-4, 319, 9, -2.92e-4, 782, 14, 3, 0]
#             keywords:  {reverse_monolayer:  true}
```

simple model language

future options under discussion

gradient within one layer

e.g. of `magnetic_moment` or `mass_density`

calculation of parameters as a function of layers underneath / above ...

e.g. for increasing `sigma` (roughness)

deuteration using the formula

e.g.
```
formula:  C6H12
deuteration:  0.4
```
gives the SLD of $C_6H_{7.2}D_{4.8}$

scaling of data base entries

e.g.
```
formula:  Fe
magnetic_moment:  2.1
rel_density:  0.9
```
scales the SLD and the magnetic_moment by 0.9

simple model language

state of the project

project web page

syntax	defined
dictionaries	advanced
tested	with simple scripts
implemented	in an `orsopy` branch

github page

`https://github.com/reflectivity/orsopy/pull/83`

this is not yet part of the specifications of `orsopy`!

→ further discussion and testing is needed.

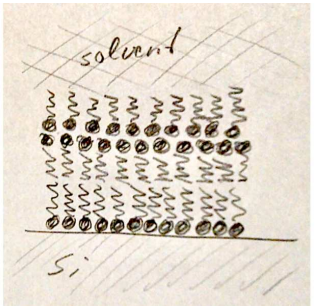
but it can already be used in the `.ort` data file.

simple model language

conclusion

simple `air | 5 ( Fe 6 | Ti 7 ) | Si`

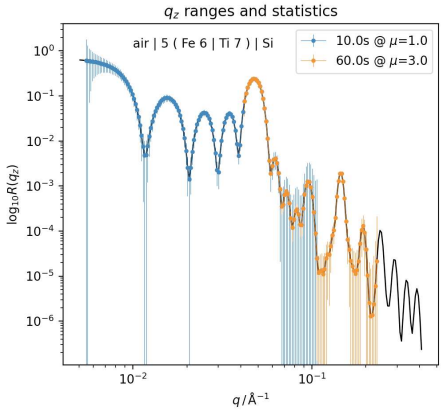
flexible



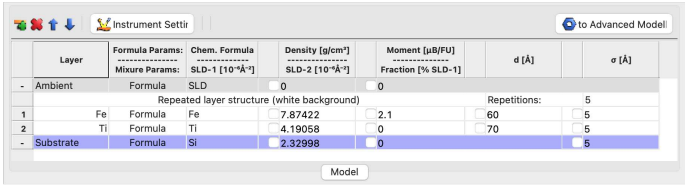
project web page

github page

experiment planning



data analysis



completeness of reflectivity file

```
model:
  origin:  NICOS input mask
  stack:  air | 5 ( Fe 6 | Ti 7 ) | Si
  globals:
    length_unit:  nm
```

indexing of data

to come

simple model language

project web page

github page

THANKS for listening

for contributing in the (near) future