20-nm-C-250-nm-ZnO-Silica-15kV-reflin-1e-1

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Abstract

The objective was to measure the time required for this simulation using the `Zn L3-M4` transition to reach the `REFLIN` criterion of an uncertainty of $1.0e^{-1}$. This was a fairly weak transition (0.1140) compared to the stronger `Zn L3-M5` transition (1.0). Still, I want to see how the simulation scales with the value of the uncertainty criterion.

Contents

Set up for the analysis

Note: This simulation used the same `MSIMPA` parameters for all layers and a `REFLIN` parameter (`1.E-1`) to finish.

```
RSEED  -10   1                [Seeds of the random-number generator]
REFLIN 30040800 1 1.E-1     [Zn L3-M4 IZ*1e6+S1*1e4+S2*1e2,dete,tol.]
NSIMSH 1.0e8                    [Desired number of simulated showers]
TIME   1.0e6                       [Allotted simulation time, in sec]
```

First load the libraries we need…

```
library(rpenepma)
library(dplyr)
library(pander)
panderOptions('table.split.table', Inf)
library(ggplot2)
library(here)
library(readr)
```

Next, set the paths and constants that we need…

```
moved_data   <- TRUE  # set to TRUE when simu is done and .rda with data is moved...
e0           <- 15 # kV
int_lo_lim   <- 1.0e-1
```

```
int_hi_lim  <- 1.0e4
reflin_crit <- 1e-1
data_dir <- here("penepma/penepma16/reflin-test/20-nm-C-250-nm-ZnO-Silica-15kV-reflin-1e-1")
# ori_sim_dir <- "C:/Users/jrminter/Documents/work/penepma16/20-nm-C-250-nm-ZnO-Silica-reflin2"
sim_nam     <- "20-nm-C-250-nm-ZnO-Silica-reflin-1e-1"
res_fi      <- sprintf("%s/%s", data_dir, "penepma-res.dat")
tim_fi      <- sprintf("%s/%s", data_dir, "delta_t.rda")
int_fi      <- sprintf("%s/%s", data_dir, "pe-intens-01.dat")
spc_fi      <- sprintf("%s/%s",data_dir, "pe-spect-01.dat")
out_ti      <- sprintf("%s-%gkV", sim_nam, e0)
msa_fi      <- sprintf("%s/%s-%gkV.msa", data_dir, sim_nam, e0)
```

Get the current simulation time

```
# When we have moved the simulation, reload the delta_t.rda
msg <- "Analyzed from data stored in delta_t.rda."
load(tim_fi)

print(msg)
```

```
[1] "Analyzed from data stored in delta_t.rda."
```

```
delta_t_time <- print(delta_t)
```

```
Time difference of 1.689805 days
```

Sort summary: this is precision overkill…

Retrieve the number of showers

We want retrieve the number of showers (trajectories) that our `penepma16` simulation calculated.

```
options(scipen = -6) # force printing in exponential format
num_showers <- penepma_get_number_of_showers(res_fi)
cat(num_showers)
```

```
1.253511e+06
```

```
options(scipen = 3) # reset to default
```

Compute the total maximum intensity for each element

Retrieve the data

First retrieve the intensity data as a `tibble` and print a preview.

```
tib <- penepma_get_intensities(int_fi)
print(tib)
```

```
# A tibble: 24 x 14
      IZ S0    S1      keV    P.mu    P.se    C.mu    C.se     B.mu
```

```
   <int> <chr> <chr> <dbl>   <dbl>   <dbl>   <dbl>   <dbl>    <dbl>
 1     6 K     L2    0.277 8.24e-7 3.66e-7 1.21e-9 2.09e-9 5.23e-10
 2     6 K     L3    0.277 1.60e-6 5.09e-7 2.42e-9 2.96e-9 4.42e-10
 3     8 K     L2    0.525 1.67e-5 7.57e-6 3.18e-8 1.94e-8 8.55e- 9
 4     8 K     L3    0.525 2.90e-5 9.28e-6 8.18e-8 3.85e-8 1.17e- 8
 5    30 L3    M1    0.884 2.77e-5 1.00e-6 1.24e-7 2.67e-7 1.12e- 7
 6    30 L2    M1    0.906 1.34e-5 6.98e-7 6.04e-9 1.24e-8 9.67e- 9
 7    30 L3    M2    0.932 8.06e-8 5.40e-8 0.      0.      1.44e-10
 8    30 L3    M3    0.934 6.04e-8 4.68e-8 0.      0.      0.
 9    30 L2    M3    0.957 6.04e-8 4.68e-8 0.      0.      0.
10    30 L3    M5    1.01  3.72e-5 1.16e-6 1.31e-7 2.67e-7 2.81e- 8
# ... with 14 more rows, and 5 more variables: B.se <dbl>, TF.mu <dbl>,
#   TF.se <dbl>, Int.mu <dbl>, Int.se <dbl>
```

What features did we measure?

```
print(names(tib))
```

```
 [1] "IZ"     "S0"     "S1"     "keV"    "P.mu"   "P.se"   "C.mu"
 [8] "C.se"   "B.mu"   "B.se"   "TF.mu"  "TF.se"  "Int.mu" "Int.se"
```

How many transitions did we measure?

```
print(nrow(tib))
```

```
[1] 24
```

Measure our test transition ("Zn L3-M4")

```
val <- penepma_get_total_intensity_z_transition(tib, 30, "L3", "M4")
print(val)
```

```
# A tibble: 1 x 7
  Symbol    IZ S0    S1         Int.mu      Int.se Int.snr
  <chr>  <int> <chr> <chr>       <dbl>       <dbl>   <dbl>
1 Zn        30 L3    M4    0.00000362 0.000000362   10.00
```

And see how close we are to the `REFLIN` criterion

```
cur_ref_crit <- val$Int.se/val$Int.mu

rv <- c(cur_ref_crit, 100*reflin_crit/cur_ref_crit)
names(rv) <-c("value", "target %")
print(rv)
```

```
     value   target %
 0.1000491 99.9509116
```

Let's estimate the remaining time

```
pct <- rv[2]/100.
names(pct) <- c()
tr <- delta_t*(1.0-pct)
print(tr)
```

```
Time difference of 0.000829498 days
```

Let's store a `.rda` file with `REFLIN` info

```
tmp_v <- data.frame(as.character(sim_nam),
                    as.numeric(reflin_crit), as.character.POSIXt(delta_t_time),
                    as.numeric(num_showers), as.numeric(cur_ref_crit),
                    as.numeric(100*reflin_crit/cur_ref_crit))
names(tmp_v) <- c("name", "reflin", "time", "showers",
                  "value", "target %")

tmp_v <- as_tibble(tmp_v)
tmp_v$name <- as.character(tmp_v$name)
C_20_nm_ZnO_250_nm_SiO2_15kV_reflin_1e_m1_ro <- tmp_v
rm(tmp_v)

save(C_20_nm_ZnO_250_nm_SiO2_15kV_reflin_1e_m1_ro,
     file="./C_20_nm_ZnO_250_nm_SiO2_15kV_reflin_1e_m1_ro.rda")
rm(C_20_nm_ZnO_250_nm_SiO2_15kV_reflin_1e_m1_ro)
load("./C_20_nm_ZnO_250_nm_SiO2_15kV_reflin_1e_m1_ro.rda")
pander(C_20_nm_ZnO_250_nm_SiO2_15kV_reflin_1e_m1_ro)
```

name	reflin	time	showers	value	target %
20-nm-C-250-nm-ZnO-Silica-reflin-1e-1	0.1	1.689805 days	1253511	0.1	99.95

Compute the maximum total intensity for each element

1. Compute the maximum total intensity for each element.
2. Stack each row of data together into a tibble.
3. Prepend the sample ID to the data.
4. Print a well-formatted a table using `pander`.
5. Save the final tibble so it can be r-loaded later

```
# 1
C_t   <- penepma_get_max_total_intensity_z(tib, 6)
O_t   <- penepma_get_max_total_intensity_z(tib, 8)
Zn_t  <- penepma_get_max_total_intensity_z(tib, 30)
Si_t  <- penepma_get_max_total_intensity_z(tib, 14)
# 2
tot_int <- dplyr::bind_rows(C_t, O_t, Zn_t, Si_t)
#3
C_20_nm_ZnO_250_nm_SiO2_15kV_reflin_1e_m1 <- prepend_sample_id_max_int_tib(tot_int, out_ti)
# 4
pander(C_20_nm_ZnO_250_nm_SiO2_15kV_reflin_1e_m1)
```

Sample.ID	Symbol	IZ	S0	S1	Int.mu	Int.se	Int.snr
20-nm-C-250-nm-ZnO-Silica-reflin-1e-1-15kV	C	6	K	L3	0.000001599	0.000000509	3.141
20-nm-C-250-nm-ZnO-Silica-reflin-1e-1-15kV	O	8	K	L3	0.00002905	0.00000928	3.13
20-nm-C-250-nm-ZnO-Silica-reflin-1e-1-15kV	Zn	30	L3	M5	0.00003732	0.00000119	31.36
20-nm-C-250-nm-ZnO-Silica-reflin-1e-1-15kV	Si	14	K	L3	0.00004103	0.0000181	2.267

```
# 5
save(C_20_nm_ZnO_250_nm_SiO2_15kV_reflin_1e_m1,
     file="C_20_nm_ZnO_250_nm_SiO2_15kV_reflin_1e_m1.rda")
# delete and reload be sure it worked...
rm(C_20_nm_ZnO_250_nm_SiO2_15kV_refli2n)
load("./C_20_nm_ZnO_250_nm_SiO2_15kV_reflin_1e_m1.rda")
```

Process the spectra data

Load the raw data

```
tib <- penepma_read_raw_data(spc_fi)
rownames(df) <- c()
```

Examine the start:

```
pander(head(tib))
```

keV	pd.mu	pd.unc
0.2717	1.874e-08	5.331e-09
0.2753	0.0000006844	0.0000001713
0.279	1.921e-08	6.218e-09
0.2826	2.118e-08	6.453e-09
0.2863	2.27e-08	7.288e-09
0.29	1.834e-08	6.811e-09

Examine the end:

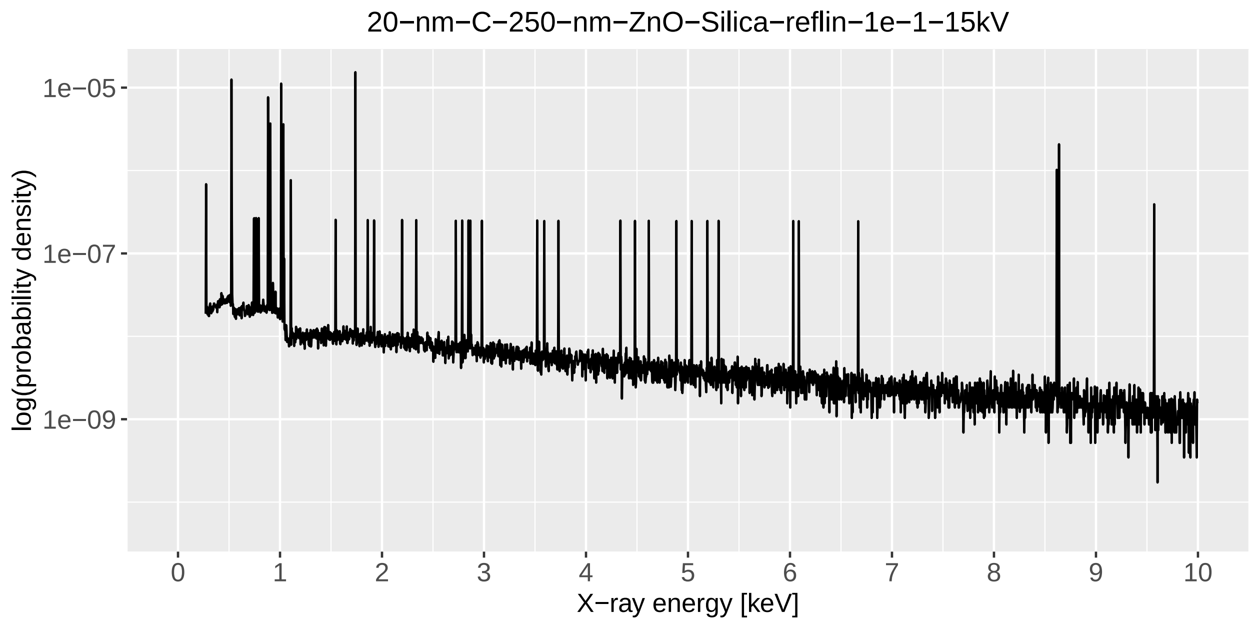
```
pander(tail(tib))
```

keV	pd.mu	pd.unc
14.88	1.726e-10	5.178e-10
14.88	1.726e-10	5.178e-10
14.89	1.726e-10	5.178e-10
14.9	3.452e-10	7.323e-10
14.96	1.726e-10	5.178e-10
14.96	1.726e-10	5.178e-10

Plot the spectrum.

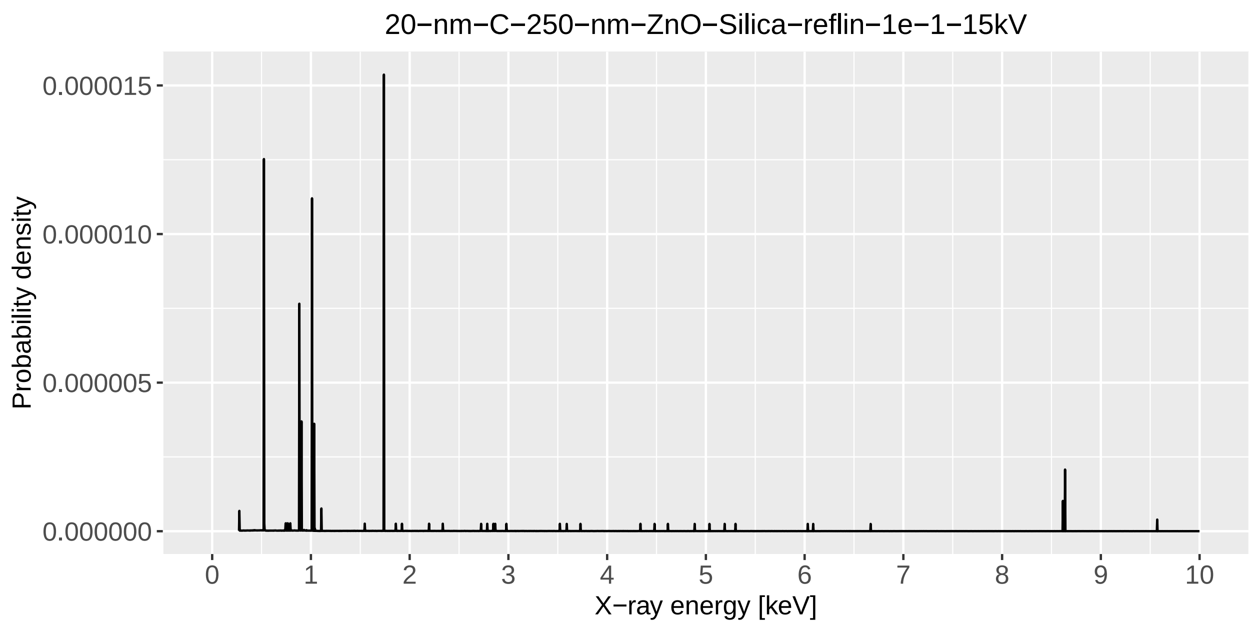
There is a very large dynamic range for both the **probability density** and the **uncertainty**. Penepma sets a lower limit for data at **1.0e-35**. Missing values are set to zero. We want to remove values from the dataframe that are below a useful limit. We do this below and plot a copy of the dataframe that is limited to the useful values.

```
m_t <- max(pretty(tib$mu))

plt <- ggplot(tib, aes(x = keV, y = pd.mu)) +
       geom_line() +
       scale_x_continuous(breaks = seq(from = 0, to = e0-5, by = 1),
                          limits = c(0,e0-5)) +
       scale_y_log10() +
       xlab(label="X-ray energy [keV]") +
       ylab(label="log(probability density)") +
       # (1/(eV*sr*electron)") +
       ggtitle(out_ti) +
       theme(axis.text=element_text(size=12),
             axis.title=element_text(size=12),
             # center the title
             plot.title = element_text(hjust = 0.5))

print(plt)
```



And on a linear intensity scale…

```
plt <- ggplot(tib, aes(x = keV, y = pd.mu)) +
       geom_line() +
       scale_x_continuous(breaks = seq(from = 0, to = e0-5, by = 1),
                          limits = c(0,e0-5)) +
       scale_y_continuous() +
       xlab(label="X-ray energy [keV]") +
       ylab(label="Probability density") +
       # (1/(eV*sr*electron)") +
       ggtitle(out_ti) +
       theme(axis.text=element_text(size=12),
             axis.title=element_text(size=12),
             # center the title
             plot.title = element_text(hjust = 0.5))

print(plt)
```



Write a spectrum file in MSA format

```
penepma_to_msa(spc_fi, msa_fi,e0, out_ti)
```