

Supplement - Les sables de Fontainebleau: A Natural Quartz Reference Sample and its Characterisation

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1 Scope

This document contains the complete data analysis undertaken for the manuscript using the statistical programming environment **R** and the package ‘Luminescence’ (version: 0.8.0). Included also are figures not shown in the main text but created for a better interpretation of the results.

2 Data import

```
rm(list = ls())
library(Luminescence)
temp <-
  read_BIN2R(
    file = "../BIN/",
    fastForward = TRUE,
    pattern = ".bin",
    txtProgressBar = FALSE,
    verbose = FALSE
  )
```

3 Data analysis

3.1 Basic summary

3.1.1 All curves

```
##get TL data for full extent plot
TL.1 <- set_RLum(class = "RLum.Analysis", records = get_RLum(temp[-11], record.id = 1))
TL.2 <- set_RLum(class = "RLum.Analysis", records = get_RLum(temp[-11], record.id = 2))
IRSL <- set_RLum(class = "RLum.Analysis", records = get_RLum(temp[-11], record.id = 3))
OSL <- set_RLum(class = "RLum.Analysis", records = get_RLum(temp[-11], record.id = 4))
TL.3 <- set_RLum(class = "RLum.Analysis", records = get_RLum(temp[-11], record.id = 5))

par(mfrow = c(1,5), cex = 1.2) #one row and five columns
plot_RLum(
  TL.1,
  combine = TRUE,
  col = rgb(0, 0, 0, 0.4),
  legend = FALSE,
  ylab = "TL [cts/\u00B0C]",
  main = "TL - initial",
  plot.single = TRUE,
  cex = 1.8,
  subs = "test",
  sub = "(5 K/s)"
)
plot_RLum(
  TL.2,
  combine = TRUE,
  col = rgb(0, 0, 0, 0.4),
  legend = FALSE,
  ylab = "TL [cts/\u00B0C]",
  main = "TL - cutheat",
  plot.single = TRUE,
  cex = 1.8,
  sub = "(5 K/s)"
)
plot_RLum(
  IRSL,
  combine = TRUE,
  col = rgb(0, 0, 0, 0.4),
  legend = FALSE,
  ylab = "IRSL [cts/0.1 s]",
  main = "IRSL",
  plot.single = TRUE,
  cex = 1.8
)
plot_RLum(
  OSL,
  combine = TRUE,
  col = rgb(0, 0, 0, 0.4),
  legend = FALSE,
  ylab = "OSL [cts/0.1 s]",
```

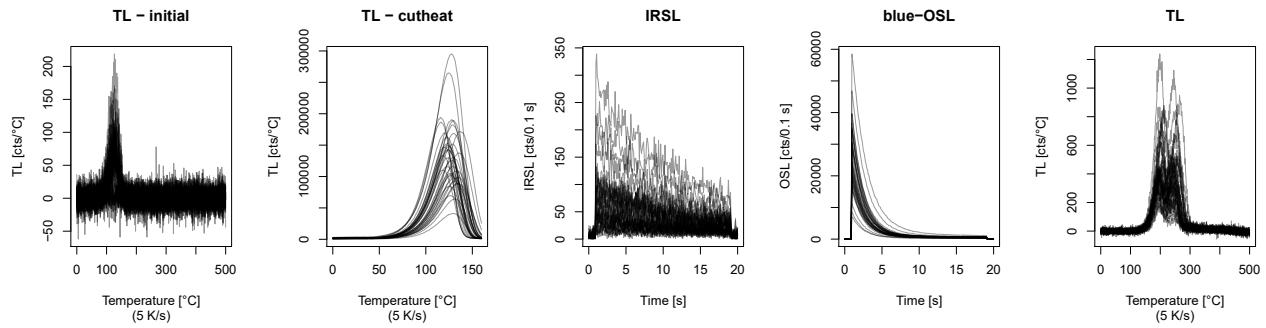


Figure S1: For a description see Figure 7 in the main text.

```

main = "blue-OSL",
plot.single = TRUE,
cex = 1.8
)
plot_RLum(
  TL.3,
  combine = TRUE,
  col = rgb(0, 0, 0, 0.4),
  legend = FALSE,
  ylab = "TL [cts/\u00B0C]",
  main = "TL",
  plot.single = TRUE,
  cex = 1.8,
  sub = "(5 K/s)"
)

```

3.1.2 Single curves - selection

```

id <- c(seq(1, length(temp), by = 2))

for(i in 1:length(id)){

##get TL data
TL.1_single <- set_RLum(
  class = "RLum.Analysis", records = get_RLum(temp[c(id[i], id[i] + 1)], record.id = 1))
TL.2_single <- set_RLum(
  class = "RLum.Analysis", records = get_RLum(temp[c(id[i], id[i] + 1)], record.id = 2))
IRSL_single <- set_RLum(
  class = "RLum.Analysis", records = get_RLum(temp[c(id[i], id[i] + 1)], record.id = 3))

##exception if
if(id[i] == 11){
  OSL_single <- set_RLum(class = "RLum.Analysis",
    records = get_RLum(temp[id[i] + 1], record.id = 4))
  TL.3_single <- set_RLum(class = "RLum.Analysis",
    records = get_RLum(temp[id[i] + 1], record.id = 5))
}else{
  OSL_single <- set_RLum(

```

```

        class = "RLum.Analysis",
        records = get_RLum(temp[c(id[i], id[i] + 1)], record.id = 4))
    TL.3_single <- set_RLum(
        class = "RLum.Analysis",
        records = get_RLum(temp[c(id[i], id[i] + 1)], record.id = 5))

}

##print
if(i <= 20){
  file_name <- paste0("FB",i,"A")

}else{
  file_name <- paste0("FB",i,"B")
}

par(mfrow = c(1,5), cex = 1.2)
plot_RLum(
  TL.1_single,
  combine = TRUE,
  legend = TRUE,
  legend = FALSE,
  mtext = file_name,
  main = "TL - initial",
  plot.single = TRUE,
  cex = 1.8,
  sub = "(5 K/s)"
)

plot_RLum(
  TL.2_single,
  combine = TRUE,
  legend = FALSE,
  mtext = file_name,
  main = "TL - cutheat",
  plot.single = TRUE,
  cex = 1.8,
  sub = "(5 K/s)"
)

plot_RLum(
  IRSL_single,
  combine = TRUE,
  legend = FALSE,
  mtext = file_name,
  main = "IRSL",
  plot.single = TRUE,
  cex = 1.8
)

plot_RLum(
  OSL_single,

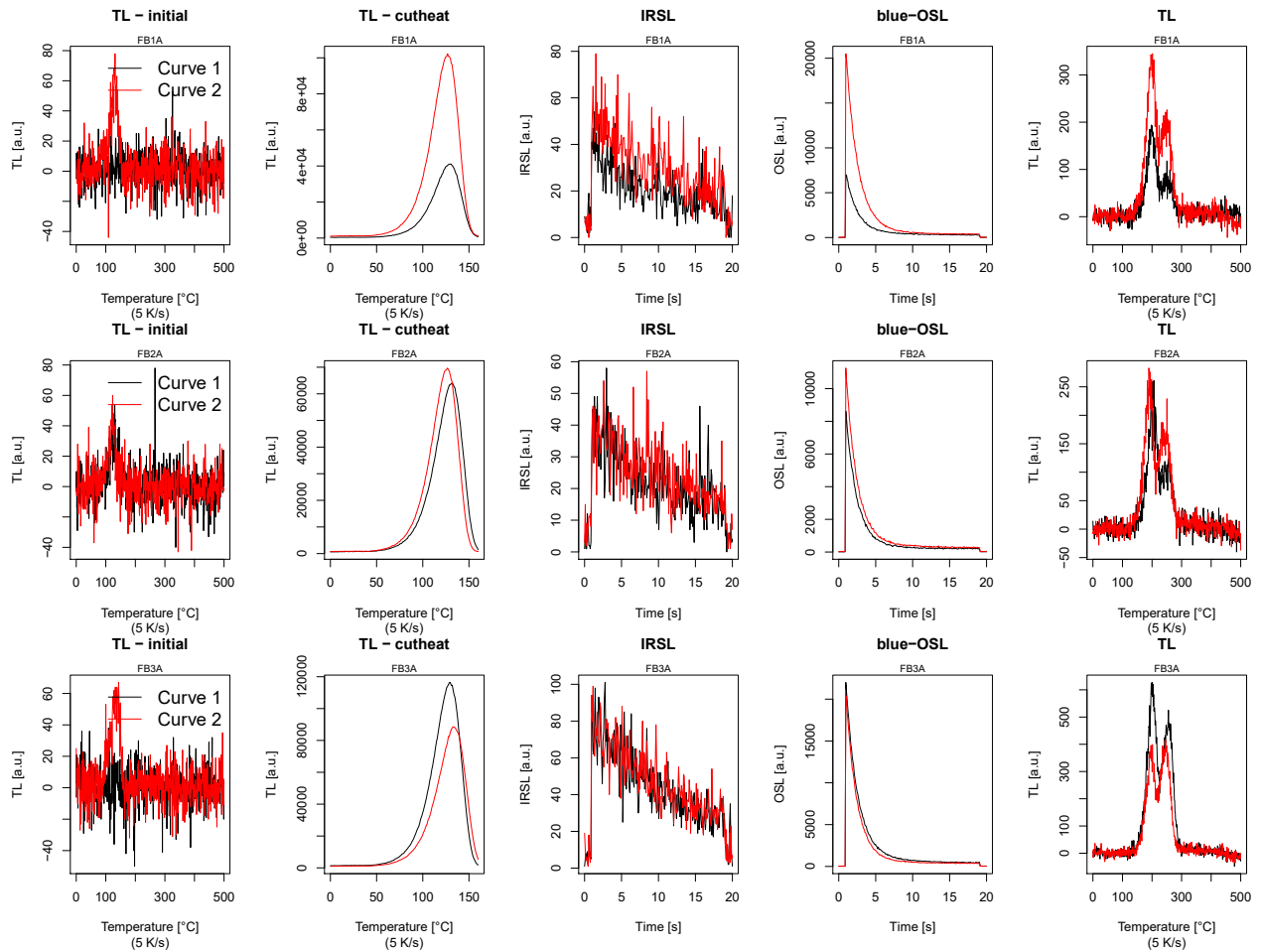
```

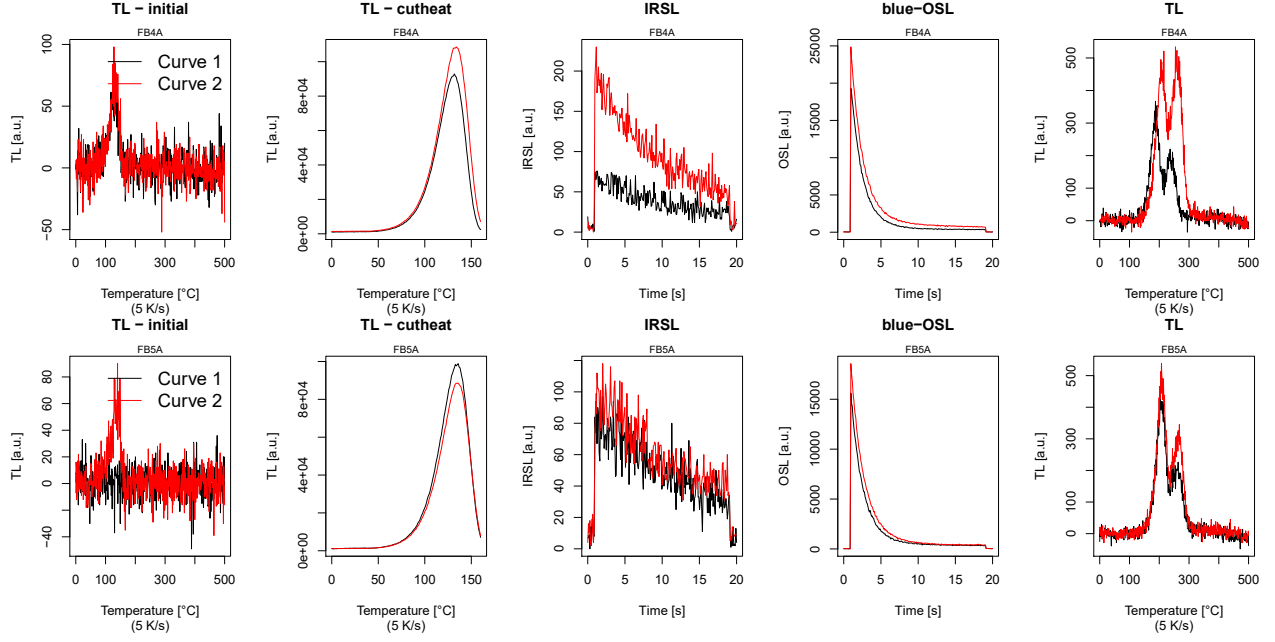
```

combine = TRUE,
legend = FALSE,
mtext = file_name,
main = "blue-OSL",
plot.single = TRUE,
cex = 1.8
)

plot_RLum(
  TL.3_single,
  combine = TRUE,
  legend = FALSE,
  mtext = file_name,
  main = "TL",
  plot.single = TRUE,
  cex = 1.8,
  sub = "(5 K/s)"
)
}

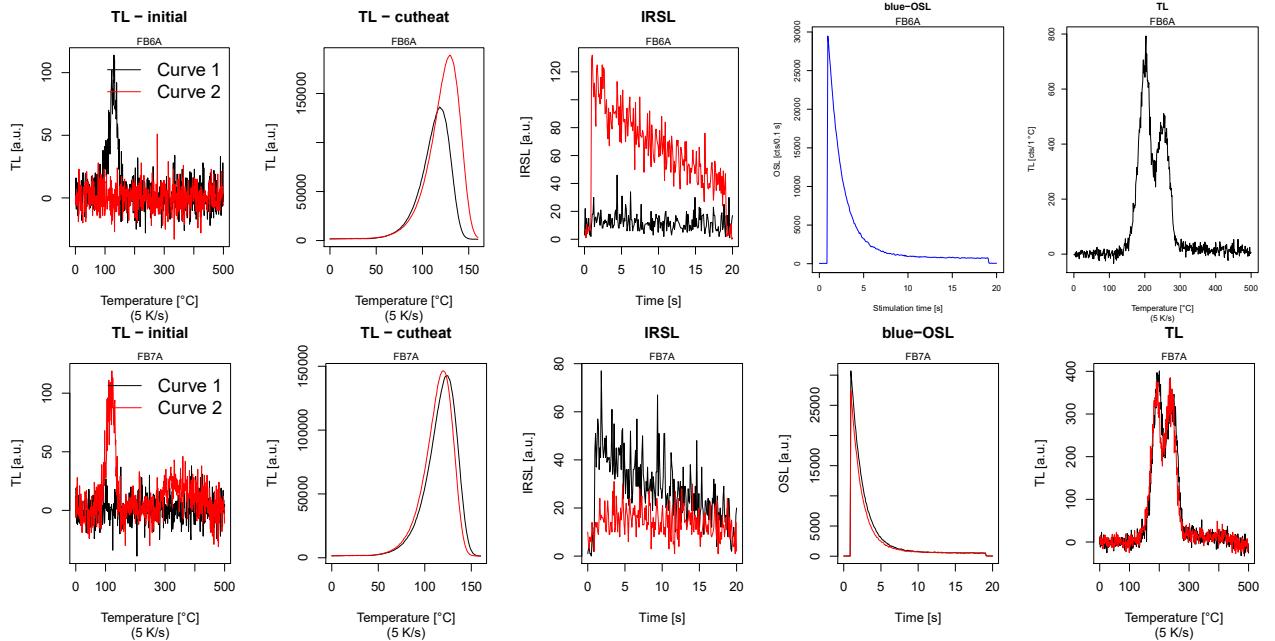
```

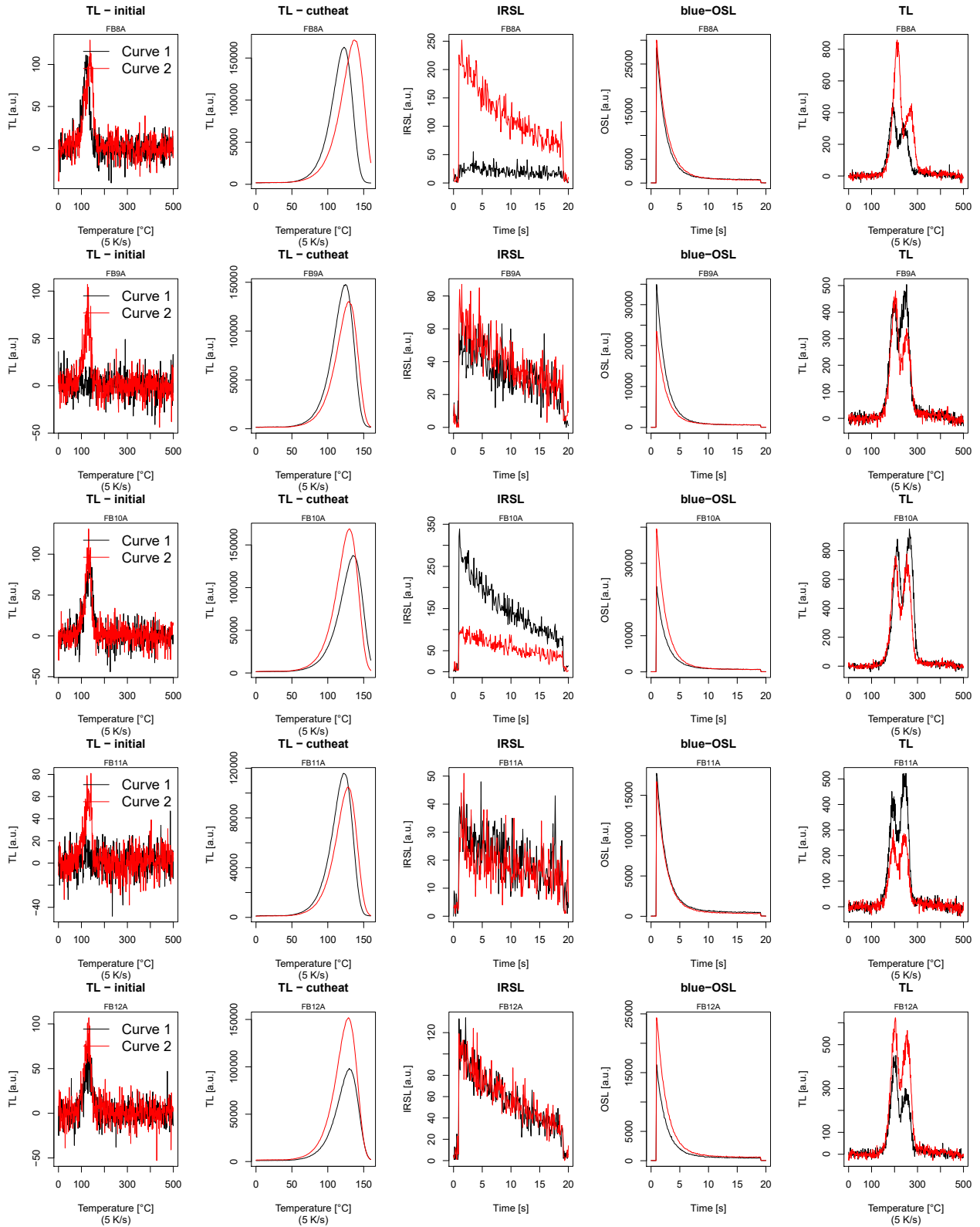


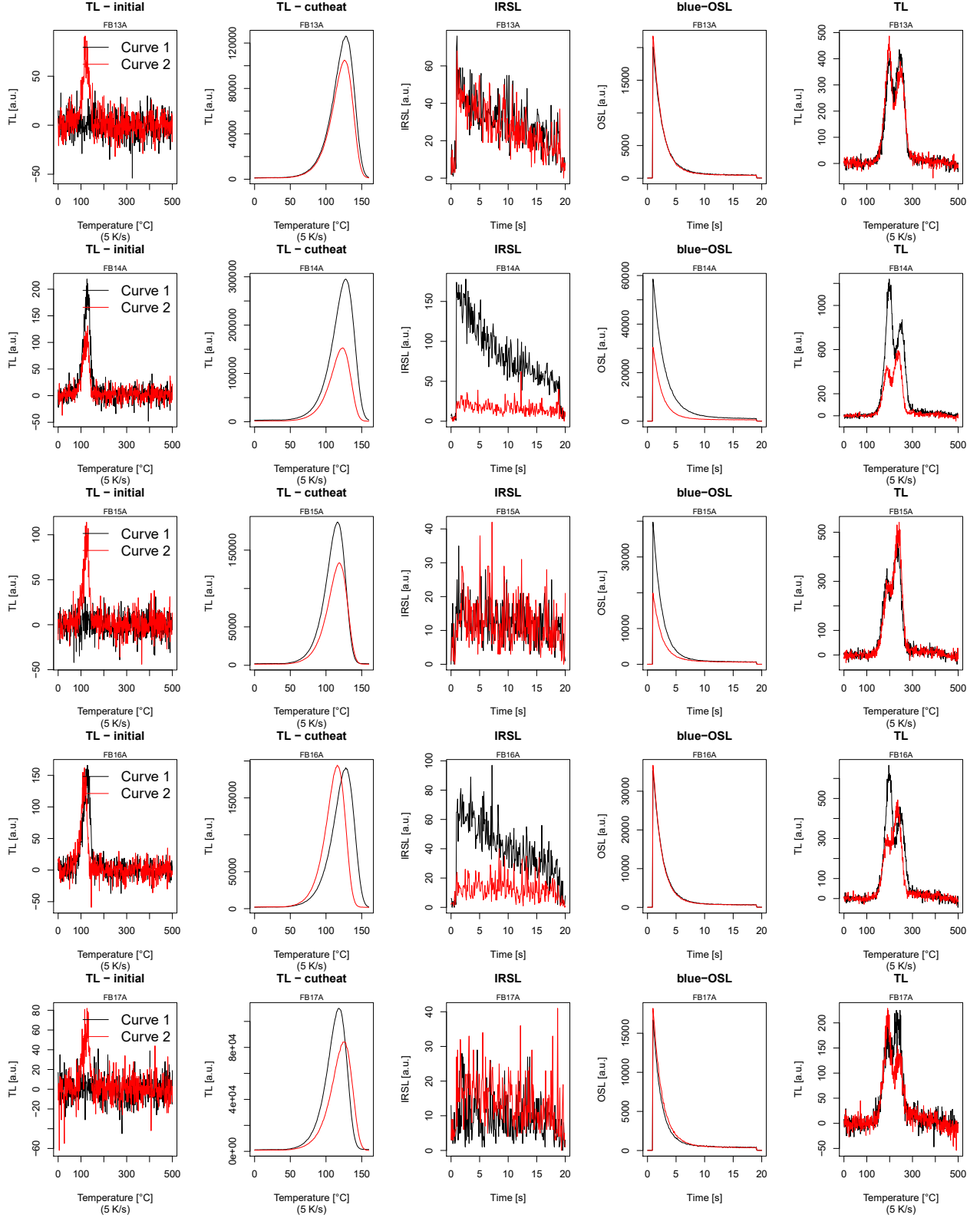


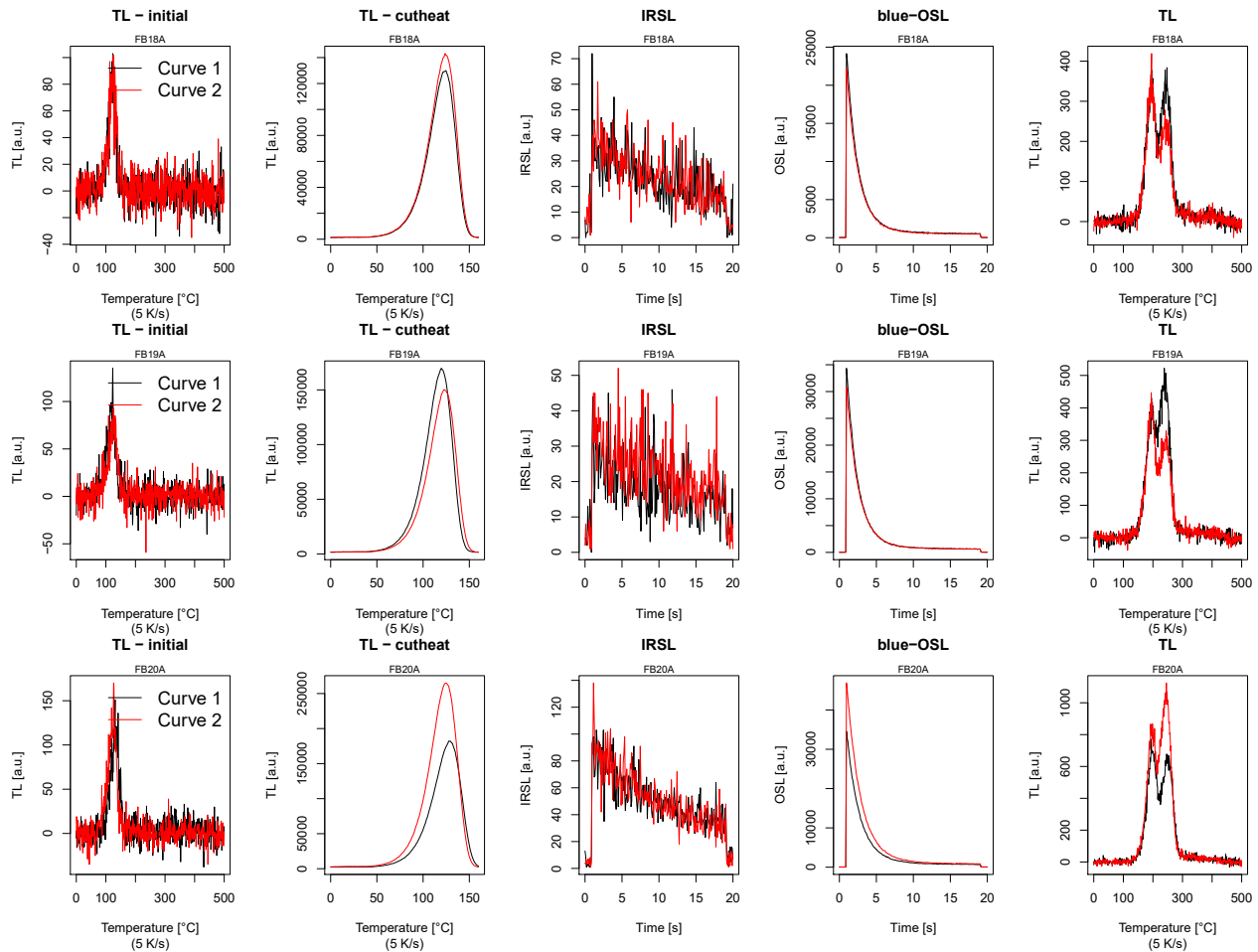
```
## Warning in plot_RLum.Analysis(object = object, subset = NULL, ...): Nothing
## to combine, object contains a single curve.
```

```
## Warning in plot_RLum.Analysis(object = object, subset = NULL, ...): Nothing
## to combine, object contains a single curve.
```









3.2 Further analyses

3.2.1 Calculate base values

```
##Histogram plots ... what do we need?
## - 110 C peak ... an the integral 5 deg to the left an to the right
TL_intensity <- unlist(lapply(get_RLum(TL.2), function(x){
  ##get index and sum
  id <- which.max(get_RLum(x)[,2])
  sum(get_RLum(x)[(id-5):(id+5),2])
}))

##IRSL intensity
IRSL_intensity <- unlist(lapply(get_RLum(IRSL), function(x){
  sum(get_RLum(x)[11:20,2])
}))

##OSL intensity
OSL_intensity <- unlist(lapply(get_RLum(OSL), function(x){
  sum(get_RLum(x)[11:20,2])
}))
```

```

}))

##get low TL peak
TL_intensity_3_low <- unlist(lapply(get_RLum(TL.3), function(x){
  ##get index and sum
  id <- which.max(get_RLum(x)[1:220,2])
  sum(get_RLum(x)[(id-5):(id+5),2])

}))

#get high TL peak
TL_intensity_3_high <- unlist(lapply(get_RLum(TL.3), function(x){
  ##get index and sum
  id <- which.max(get_RLum(x)[230:500,2])
  sum(get_RLum(x)[(id+230-5):(id+5),2])

}))

```

3.2.1.1 Normalised OSL/IRSL curves

```

## Add normalised plots
par(mfrow = c(1,2))
plot_RLum(
  IRSL,
  combine = TRUE,
  col = rgb(0, 0, 0, 0.4),
  legend = FALSE,
  ylab = "norm. IRSL [cts/0.1 s]",
  main = "IRSL",
  plot.single = TRUE,
  cex = 1,
  log = "x",
  norm = TRUE
)
plot_RLum(
  OSL,
  combine = TRUE,
  col = rgb(0, 0, 0, 0.4),
  legend = FALSE,
  ylab = "norm. OSL [cts/0.1 s]",
  main = "blue-OSL",
  plot.single = TRUE,
  cex = 1,
  log = "x",
  norm = TRUE
)

```

3.2.1.2 Correlation IRSL vs OSL

```

##plot
plot(OSL_intensity, IRSL_intensity,
      xlab = "OSL intensity [a.u.]",

```

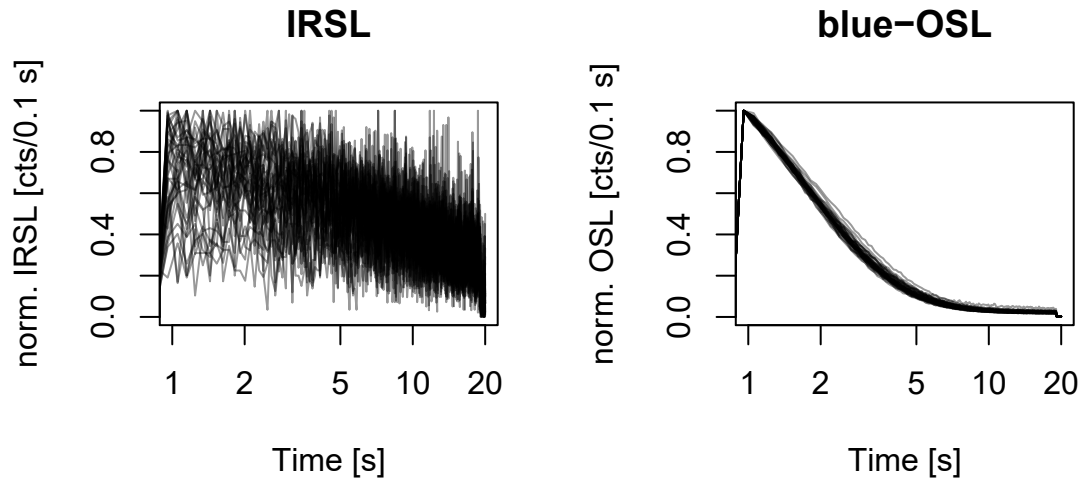


Figure S2: Normalised IRSL (left) and OSL (right) curves. All curves are normalised to the first channel each. IRSL curve shapes are hardly distinguishable due to the low signal intensity. OSL curve shapes are similar, except for a few outliers, which indicate a slightly slower signal decay. Whether the observed differences result from the measurement setup or is caused by mineral inclusions within the quartz cannot be stated with certainty.

```
ylab = "IRSL intensity [a.u.]",
main = "OSL vs IRSL Signal Intensity"
)
mtext(side = 3, paste("r = ", round(cor(OSL_intensity, IRSL_intensity), 2)))
abline(lm(y ~ x, data = data.frame(x = OSL_intensity, y = IRSL_intensity)), col = "red", lty = 2)
```

3.2.1.3 IRSL/OSL ratio

```
## show IRSL/OSL ratio
boxplot(
  x = IRSL_intensity/OSL_intensity * 100,
  main = "IRSL - blue-OSL Intensity Ratio",
  ylab = "Ratio [%]"
)
abline(h = 1, col = "red")
```

3.2.2 110°C TL peak analysis

```
##scatter plot
par(mfrow = c(1,4), cex = 1.2)

plot_RLum(
  TL.2,
  combine = TRUE,
  col = rgb(0, 0, 0, 0.4),
  legend = FALSE,
  ylab = "TL [cts/\u00B0C]",
  main = "TL Peak Selection",
  plot.single = TRUE,
```

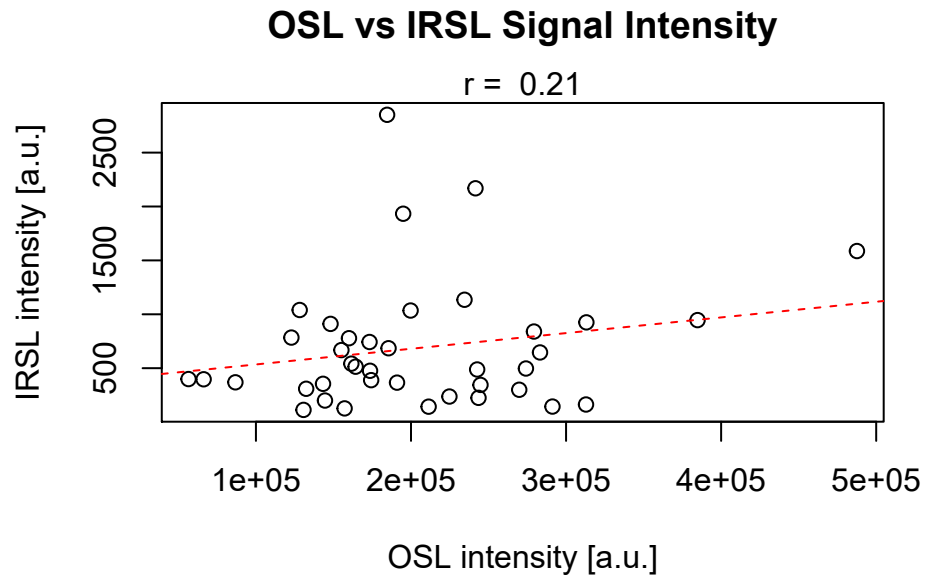


Figure S3: Shown are summed OSL signals against summed IRSL signals per measured aliquot. The plot displays only a weak correlation between the two signals. Thus the IRSL signal intensity is not linked to the OSL signal intensity, indicating that the (weak) IRSL signal originates from feldspar mineral phases within the sample.

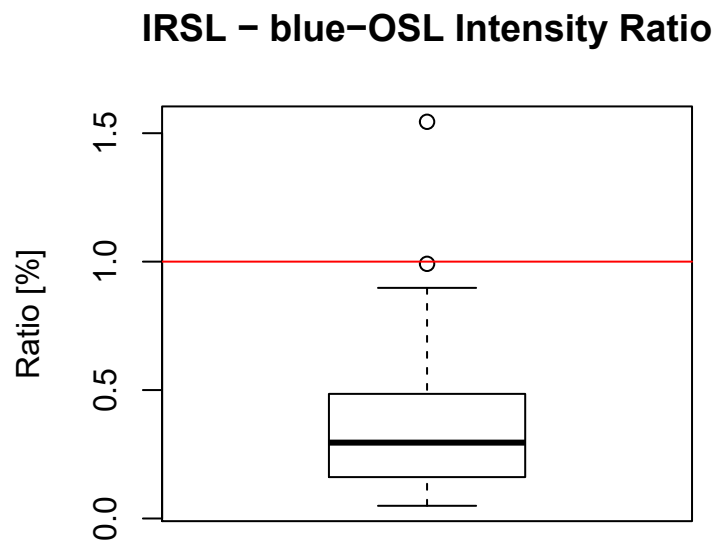


Figure S4: IRSL vs. OSL intensity ratio. Except for one outlier the ratio never exceeds 1%.

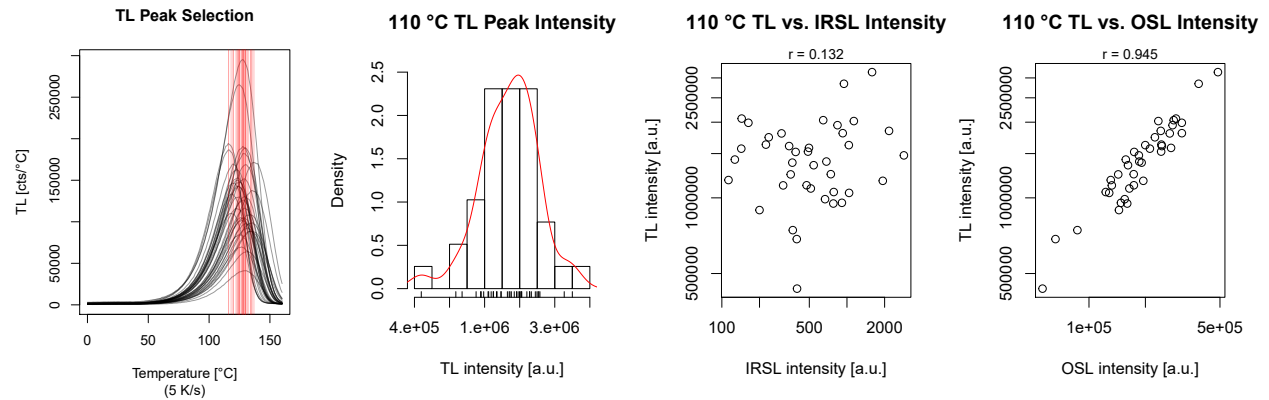


Figure S5: See Fig. 9 and its figure caption in the main text.

```

    cex = 1,
    sub = "(5 K/s)"
  )

  abline(v = sapply(get_RLum(TL.2), function(x){which.max(x[,2])}),
         col = rgb(1,0,0,0.2))

  hist(log10(TL_intensity), main = "110 °C TL Peak Intensity",
       xaxt = "n", freq = FALSE,
       xlab = "TL intensity [a.u.]", ylim = c(0,2.5))
  lines(density(log10(TL_intensity)), col = "red")
  rug(x = log10(TL_intensity))
  axis(side = 1, at = axTicks(side = 1),
       labels = format(10^axTicks(side = 1), digits = 0))

  plot(IRSL_intensity, TL_intensity,
       main = "110 °C TL vs. IRSL Intensity", log = "xy",
       ylab = "TL intensity [a.u.]",
       xlab = "IRSL intensity [a.u.]")

  mtext(side = 3, paste0("r = ", round(cor(log10(IRSL_intensity),
                                           log10(TL_intensity)), 3)))

  plot(OSL_intensity, TL_intensity,
       main = "110 °C TL vs. OSL Intensity",
       log = "xy",
       ylab = "TL intensity [a.u.]",
       xlab = "OSL intensity [a.u.]")

  mtext(side = 3, paste0("r = ", round(cor(log10(OSL_intensity),
                                           log10(TL_intensity)), 3)))

  peaks <- sapply(get_RLum(TL.2), function(x){x[which.max(x[,2]),1]})

  ##return additional information on the peak itself
  hist(x = peaks,

```

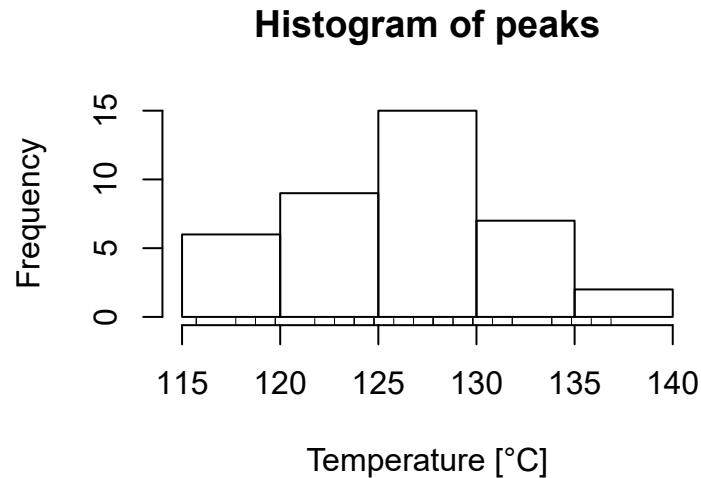


Figure S6: Histogram showing the temperature variation of the first TL peak.

```
xlab = "Temperature [\u00B0C]"
rug(peaks)
```

```
print(mean(peaks), digits = 1)
```

```
## [1] 127
```

```
print(range(peaks), digits = 1)
```

```
## [1] 116 137
```

3.2.3 200°C TL peak analysis

```
##scatter plot
par(mfrow = c(1,4), cex = 1.2)

plot_RLum(
  TL.3,
  combine = TRUE,
  col = rgb(0, 0, 0, 0.4),
  legend = FALSE,
  ylab = "TL [cts/\u00B0C]",
  main = "TL peak selection",
  plot.single = TRUE,
  cex = 1,
  sub = "(5 K/s)"
)

abline(v = sapply(get_RLum(TL.3), function(x){which.max(x[1:220,2])}),
       col = rgb(1,0,0,0.2))

hist(log10(TL_intensity_3_low),
     main = "200 \u00B0C TL peak intensity", xaxt = "n",
     freq = FALSE, xlab = "TL intensity [a.u.]")
lines(density(log10(TL_intensity_3_low)), col = "red")
```

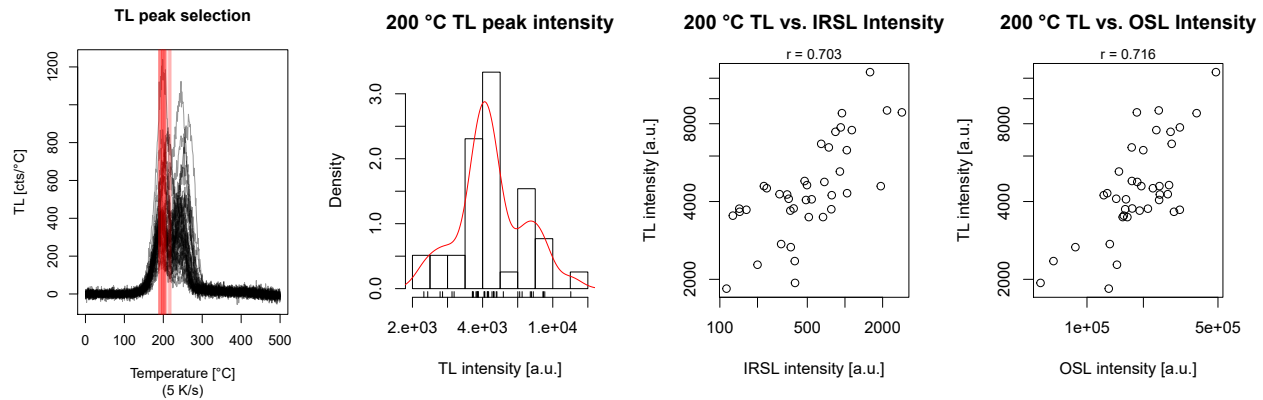


Figure S7: See Fig. 10 and its figure caption in the main text.

```
rug(x = log10(TL_intensity_3_low))
axis(side = 1, at = axTicks(side = 1),
     labels = format(10^axTicks(side = 1), digits = 0))

plot(
  IRSL_intensity,
  TL_intensity_3_low,
  main = "200 °C TL vs. IRSL Intensity",
  log = "xy",
  ylab = "TL intensity [a.u.]",
  xlab = "IRSL intensity [a.u.]"
)

mtext(side = 3, paste0("r = ", round(cor(log10(IRSL_intensity),
                                         log10(TL_intensity_3_low)), 3)))

plot(
  OSL_intensity,
  TL_intensity_3_low,
  main = "200 °C TL vs. OSL Intensity",
  log = "xy",
  ylab = "TL intensity [a.u.]",
  xlab = "OSL intensity [a.u.]"
)

mtext(side = 3, paste0("r = ", round(cor(log10(OSL_intensity),
                                         log10(TL_intensity_3_low)), 3)))
```

```
peaks <- sapply(get_RLum(TL.3), function(x){x[which.max(x[1:220,2]),1]})
```

```
##return additional information on the peak itself
```

```
hist(x = peaks,
     xlab = "Temperature [°C]")
rug(peaks)
```

```
print(mean(peaks), digits = 1)
```

```
## [1] 200
```

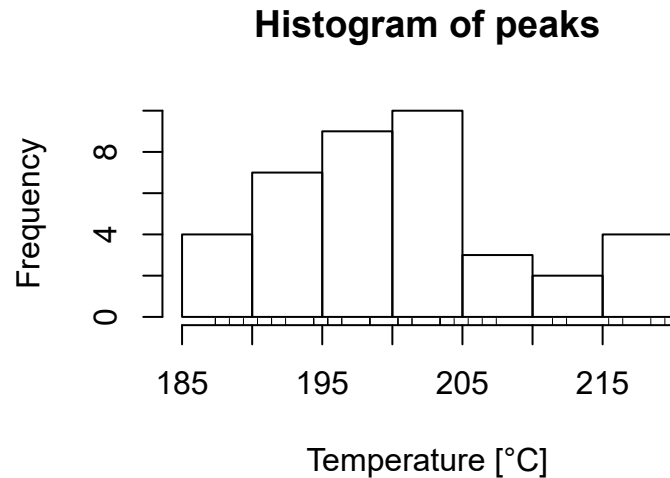


Figure S8: Histogram of temperature position variation of the 2nd TL peak.

```
print(range(peaks), digits = 1)
```

```
## [1] 187 219
```

3.2.4 250°C TL peak analysis

```
##scatter plot
par(mfrow = c(1,4), cex = 1.2)

plot_RLum(
  TL.3,
  combine = TRUE,
  col = rgb(0, 0, 0, 0.4),
  legend = FALSE,
  ylab = "TL [cts/\u00B0C]",
  main = "TL Peak Selection",
  plot.single = TRUE,
  cex = 1,
  sub = "(5 K/s)"
)

abline(v = sapply(get_RLum(TL.3), function(x){which.max(x[230:500,2]) + 230}),
       col = rgb(1,0,0,0.2))

hist(log10(TL_intensity_3_high),
     main = "250 \u00B0C TL Peak Intensity", xaxt = "n",
     freq = FALSE, xlab = "TL intensity [a.u.]")
lines(density(log10(TL_intensity_3_high)), col = "red")
rug(x = log10(TL_intensity_3_high))
axis(side = 1, at = axTicks(side = 1),
     labels = format(10^axTicks(side = 1), digits = 0))

plot(
  IRSL_intensity,
```

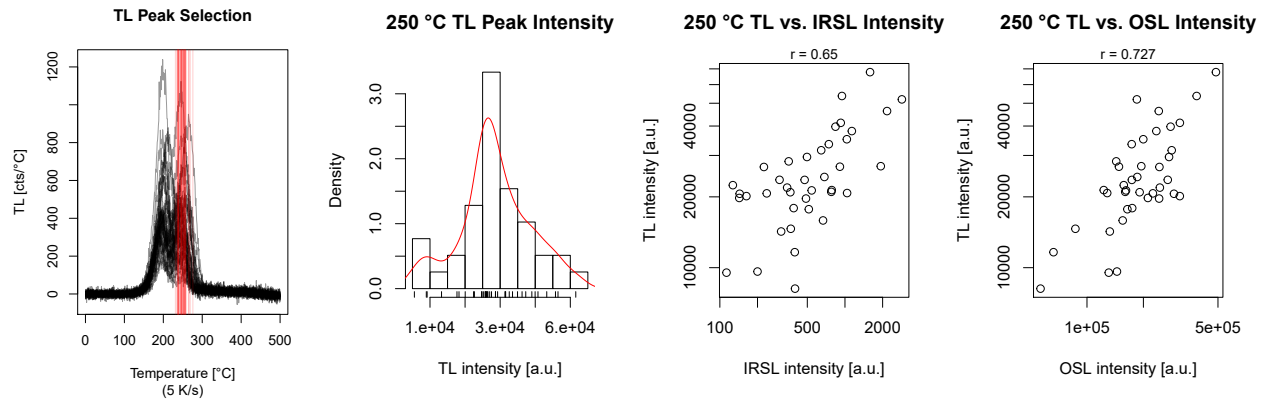



Figure S9: See Fig. 11 in its figure caption in the main text.

```

TL_intensity_3_high,
main = "250 \u00B0C TL vs. IRSL Intensity",
log = "xy",
ylab = "TL intensity [a.u.]",
xlab = "IRSL intensity [a.u.]"
)

mtext(side = 3, paste0("r = ", round(cor(log10(IRSL_intensity),
                                         log10(TL_intensity_3_high))), 3)))

plot(
  OSL_intensity,
  TL_intensity_3_high,
  main = "250 \u00B0C TL vs. OSL Intensity",
  log = "xy",
  ylab = "TL intensity [a.u.]",
  xlab = "OSL intensity [a.u.]"
)

mtext(side = 3, paste0("r = ", round(cor(log10(OSL_intensity),
                                         log10(TL_intensity_3_high))), 3)))

peaks <- sapply(get_RLum(TL.3), function(x){x[which.max(x[230:500,2]) + 230,1]})

##return additional information on the peak itself
hist(x = peaks,
     xlab = "Temperature [\u00B0C]")
rug(peaks)

print(mean(peaks), digits = 1)

## [1] 248

print(range(peaks), digits = 1)

## [1] 230 276

```

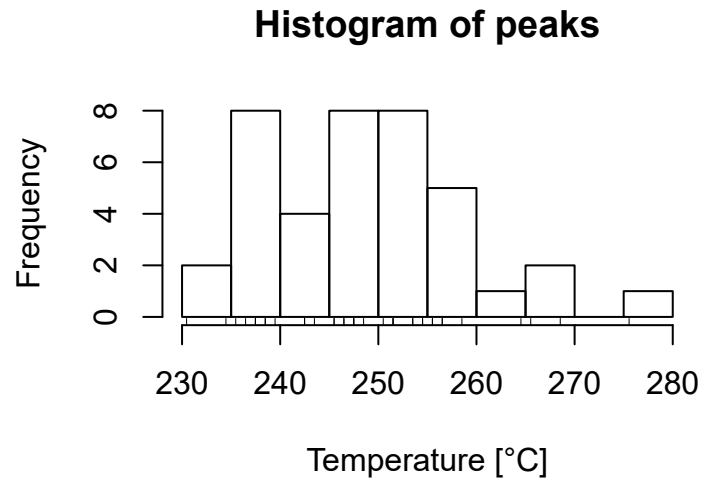


Figure S10: Histogram of the temperature variation of the upper TL peak.

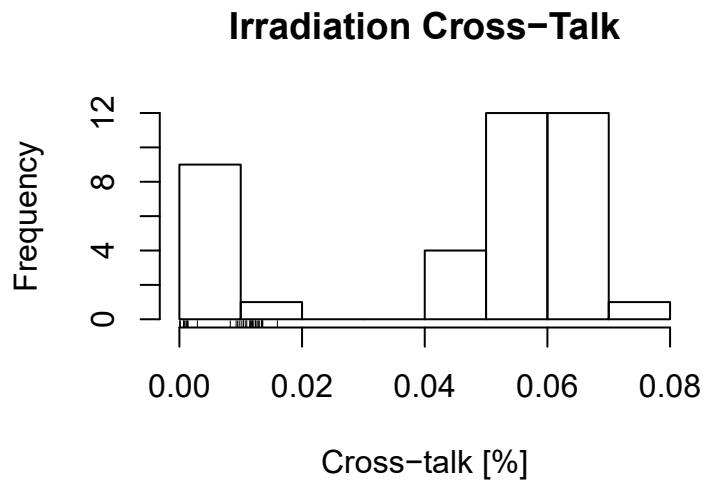


Figure S11: Histogram of the observed irradiation cross-talk.

3.2.5 Irradiation cross-talk estimation

```
##calculate the irradiation cross-talk using
##the intergral of the two TL curves up to channel 160
cross_talk <- vapply(1:length(TL.1), function(x){
  (sum(TL.1@records[[x]][1:160,2]) * 20) /
  sum(TL.2@records[[x]][,2])
}, numeric(1))

##plot in %
hist(cross_talk/20 * 100, xlab = "Cross-talk [%]", main = "Irradiation Cross-Talk")
rug(cross_talk)

##print cross-talk in different units
##print cross-talk in seconds
print(paste0(round(mean(cross_talk), 3), " ± ", round(sd(cross_talk), 3), " s"))
```

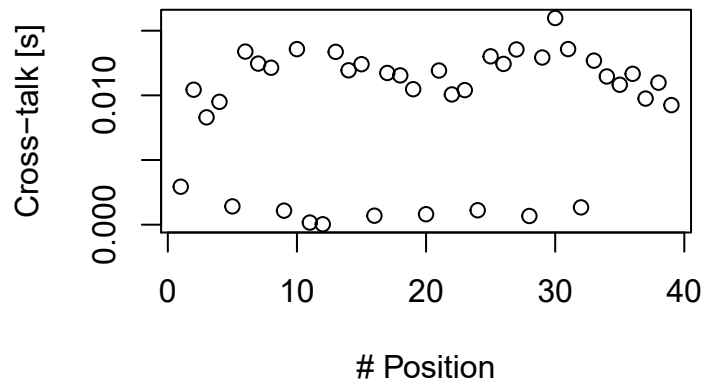


Figure S12: Observed absolute irradiation cross-talk per position.

```
## [1] "0.009 ± 0.005 s"
```

```
print(paste0(round(mean(cross_talk / 20 * 100), 3), " ± ",
              round(sd(cross_talk / 20 * 100), 3), " %"))
```

```
## [1] "0.045 ± 0.025 %"
```

```
print(paste0(
  round(mean(cross_talk) * 0.1 * 1e+6 / 2, 2),
  " ± ",
  round(sd(cross_talk) * 0.1 * 1e+6 / 2, 2),
  " µGy/Gy"
))
```

```
## [1] "451.28 ± 248.92 µGy/Gy"
```

```
##cross check position against cross_talk
plot(1:length(cross_talk),
     cross_talk,
     xlab = "# Position",
     ylab = "Cross-talk [s]")
```