Package 'RLumModel'

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RLumModel-package

Modelling Ordinary Differential Equations Leading to Luminescence

Description

A collection of function to simulate luminescence signals in the mineral quartz based on published models.

Details

Package: RLumModel Type: Package Version: 0.1.0

Date: 2016-XX-XX License: GPL-3

Author(s)

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Project source code repository

https://github.com/R-Lum/RLumModel

Related projects

http://www.r-luminescence.de

http://cran.r-project.org/package=Luminescence

http://shiny.r-luminescence.de

http://cran.r-project.org/package=RLumShiny

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```
model_LuminescenceSignals
```

Model Luminescence Signals

Description

This function models luminescence signals for quartz based on published physical models. It is possible to simulate TL, (CW-) OSL, RF measurements in a arbitrary sequence. This sequence is definded as a list of certain abrivations. Furthermore it is possible to load a sequence direct from the Riso Sequence Editor. The output is an RLum.Analysis object and so the plots are done by the plot_RLum.Analysis function. If a SAR sequence is simulated the plot output can be disabled and SAR analyse functions can be used.

Usage

```
model_LuminescenceSignals(model, sequence, lab.DoseRate = 1,
    simulate_sample_history = FALSE, plot = TRUE, verbose = TRUE, ...)
```

Arguments

mode1 character (required): set model to be used list (required): set sequence to model as list or as *.seq file from the Riso sequence sequence editor. To simulate SAR measurements there is an extra option to set the sequence list (cf. example 3): (required): RegDose: numeric, Test-Dose: numeric, PH: numeric, CH: numeric, OSL_temp: numeric. With default are: DoseRate: numeric, Irr_temp: numeric, optical_power: numeric, OSL_duration: numeric, PH_duration: numeric lab.DoseRate numeric (with default): laboratory dose rate in XXX Gy/s for calculating seconds into Gray in the *.seq file. simulate_sample_history logical (with default): FALSE (with default): simulation begins at labour conditions, TRUE: simulations begins at crystallization (all levels 0) process logical (with default): Enables or disables plot output plot verbose logical (with default): Verbose mode on/off further arguments and graphical parameters passed to plot.default. See details for further information

Details

Defining a sequence

Abrivation	Description	Arguments
TL	thermally stimulated luminescence	'temp begin', 'temp end', 'heating rate'
OSL	optically stimulated luminescence	'temp', 'duration','optical power'
LM_OSL	linear modulated OSL	'temp', 'duration'

RL/RF	radioluminescence	'temp', 'dose', 'doserate'
IRR	irradiation	'temp','dose', 'doserate'
CH	cutheat	'temp', 'duration'
PH	preheat	'temp', 'duration'
PAUSE	pause	'temp', 'duration'

Value

This function returns an RLum.Analysis object with all TL, (LM-) OSL and RF/RL steps in the sequence. Every entry is a RLum.Data.Curve obejct and can be plotted, analysed etc. with further RLum functions.

Function version

0.1.0

Note

This function can do just nothing at the moment.

Author(s)

Johannes Friedrich, University of Bayreuth (Germany), Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne (France)

References

Bailey, R.M., 2001. Towards a general kinetic model for optically and thermally stimulated luminescence of quartz. Radiation Measurements 33, 17-45.

Bailey, R.M., 2002. Simulations of variability in the luminescence characteristics of natural quartz and its implications for estimates of absorbed dose. Radiation Protection Dosimetry 100, 33-38.

Bailey, R.M., 2004. Paper I-simulation of dose absorption in quartz over geological timescales and it simplications for the precision and accuracy of optical dating. Radiation Measurements 38, 299-310.

Pagonis, V., Chen, R., Wintle, A.G., 2007: Modelling thermal transfer in optically stimulated luminescence of quartz. Journal of Physics D: Applied Physics 40, 998-1006.

Pagonis, V., Wintle, A.G., Chen, R., Wang, X.L., 2008. A theoretical model for a new dating protocol for quartz based on thermally transferred OSL (TT-OSL). Radiation Measurements 43, 704-708.

See Also

plot

Examples

```
##================================##
## Example 1: Simulate sample history of Bailey2001
## (cf. Bailey, 2001, Fig. 1)
##=============================##
```

```
##set sequence with the following steps
## (1) Irradiation at 20 deg. C with a dose of 10 Gy and a dose rate of 1 Gy/s
## (2) TL from 20-400 deg. C with a rate of 5 K/s
sequence <-
  list(
   IRR = c(20, 10, 1),
   TL = c(20, 400, 5)
  )
##model sequence
model.output <- model_LuminescenceSignals(</pre>
  sequence = sequence,
  model = "Bailey2001",
## Not run:
## Example 2: Simulate sequence at labour without sample history
##set sequence with the following steps
## (1) Irraditation at 30 deg. C with a dose of 100 Gy and a dose rate of 1 Gy/s
## (2) Preheat to 2000 deg. C and hold for 10 s
## (3) LM-OSL at 125 deg. C. for 1000 s
## (4) OSL at 20 deg. C for 100 s with 90 % optical power
## (5) Cutheat at 220 deg. C
## (6) Irradiation at 20 deg. C with a dose of 10 Gy and a dose rate of 1 Gy/s
## (7) Pause at 200 deg. C for 100 s
## (8) TL from 20-400 deg. C with a heat rate of 5 K/s
## (9) Radiolumiescence at 20 deg. C with a dose of 20 Gy and a dose rate of 1 Gy/s
sequence <-
list(
  IRR = c(20, 100, 1),
  PH = c(200, 10),
  LM_{OSL} = c(125, 100),
  CH = c(200),
  IRR = c(20, 10, 1),
  PAUSE = c(200, 100),
  OSL = c(125, 100, 90),
  PAUSE = c(200, 100),
  TL = c(20, 400, 5),
  RF = c(20, 200, 0.01)
# call function "model_LuminescenceSignals", set sequence = sequence, model = "Pagonis2008" (palaeodose = 200
# and simulate_sample_history = FALSE (default), because the sample history is not part of the sequence
model.output <- model_LuminescenceSignals(</pre>
  sequence = sequence,
  model = "Pagonis2008"
##_____##
```

Example 3: Simulate SAR sequence

```
##set SAR sequence with the following steps
## (1) RegDose: set regenerative dose [Gy] as vector
## (2) TestDose: set test dose [Gy]
## (3) PH: set preheat temperature in deg. C
## (4) CH: Set cutheat temperature in deg. C
## (5) OSL_temp: set OSL reading temperature in deg. C
## (6) OSL_duration: set OSL reading duration in s
sequence <- list(</pre>
RegDose = c(0,10,20,50,90,0,10),
TestDose = 5,
PH = 240,
CH = 200,
OSL_{temp} = 125,
OSL_duration = 70
# call function "model_LuminescenceSignals", set sequence = sequence, model = "Pagonis2007" (palaeodose = 20
# and simulate_sample_history = FALSE (default), because the sample history is not part of the sequence
model.output <- model_LuminescenceSignals(</pre>
 sequence = sequence,
 model = "Pagonis2007",
plot = FALSE
# in environment is a new object "model.output" with the results of every step of the given sequence.
# Plots are done at OSL and TL steps and the growth curve
# call "analyse_SAR.CWOSL" from RLum package
 results <- analyse_SAR.CWOSL(model.output,
                          signal.integral.min = 1,
                          signal.integral.max = 15,
                          background.integral.min = 601,
                          background.integral.max = 701,
                          fit.method = "EXP",
                          dose.points = c(0,10,20,50,90,0,10))
## Example 4: generate sequence from *.seq file and run SAR simulation
##-----##
## call function "model_LuminescenceSignals", load *.seq file for sequence, set model = "Bailey2002" (palaeod
## and simulate_sample_history = FALSE (default), because the sample history is not part of the sequence
model.output <- model_LuminescenceSignals(</pre>
  sequence = "inst/extdata/sample_SAR_cycle.SEQ",
  model = "Bailey2002",
 plot = FALSE
## call RLum package function "analyse_SAR.CWOSL" to analyse the simulated SAR cycle
```

```
results <- analyse_SAR.CWOSL(model.output,
                            signal.integral.min = 1,
                            signal.integral.max = 10,
                            background.integral.min = 601,
                            background.integral.max = 701,
                            dose.points = c(0,5,10,20,50,5,0),
                            fit.method = "EXP")
print(get_RLum(results))
## Example 5: compare different optical powers of stimulation light
## call function "model_LuminescenceSignals", model = "Bailey2004"
## and simulate_sample_history = FALSE (default), because the sample history is not part of the sequence
## the optical_power of the LED is varied and then compared.
optical_power <- seq(from = 0, to = 100, by = 20)
model.output <- lapply(1:length(optical_power), function(x){</pre>
sequence \leftarrow list(IRR = c(20, 50, 1),
                 PH = c(220, 10, 5),
                 OSL = c(125, 50, optical_power[x])
return(model_LuminescenceSignals(
      sequence = sequence,
      model = "Bailey2004",
      plot = FALSE
      ))
})
##combine output curves
model.output.merged <- merge_RLum(model.output)</pre>
##plot
plot_RLum(
object = model.output.merged,
xlab = "Illumination time [s]",
ylab = "OSL signal [a.u.]",
 main = "OSL signal dependency on optical power of stimulation light",
 legend.text = paste("Optical power density", 20*optical_power/100, "mW/cm^2"),
 combine = TRUE)
## End(Not run)
```

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