Package ‘RLumModel’

December 21, 2015

Type Package

Title Modelling Ordinary Differential Equations Leading to Luminescence

Version 0.1.0

Date 2016-XX-XX

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

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License GPL-3

Depends R (>= 3.2.3), utils, Luminescence (>= 0.5.0)

Imports deSolve (>= 1.12)

URL http://CRAN.R-project.org/package=RLumModel

Collate RLumModel-package.R calc_Signal.R model_LuminescenceSignals.R plot_concentrations.R read_SEQ2R.R set_ODE.R set_ODE_LM_OSL.R set_Pars.R simulate_CW_OSL.R simulate_DRT.sequence.R simulate_LM_OSL.R simulate_RL.R simulate_SAR.sequence.R simulate_TL.R simulate_heating.R simulate_illumination.R simulate_irradiation.R simulate_pause.R translate_Sequence.R

RoxygenNote 5.0.1

Suggests testthat

NeedsCompilation no

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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

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Version:	0.1.0
Date:	2016-XX-XX
License:	GPL-3

Author(s)

Authors

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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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Acknowledgement

The work of Johannes Friedrich is gratefully supported by the DFG in framework of the project 'Modelling quartz luminescence signal dynamics relevant for dating and dosimetry' (SCHM 305114-1)

ExampleData.ModelOutput
Example data (TL curve) simulated from Bailey (2001 ,fig. 1)

Description

Example data (TL curve) simulated from Bailey (2001 ,fig. 1)

Format

A RLum.Analysis object containing one TL curve as RLum.Data.Curve.

Note

This example has only one record (TL). The used sequence was sequence <- list(IRR = c(temp = 20, dose = 10, DoseRate = 1), TL = c(temp_begin = 20, temp_end = 400, heating_rate = 5))

Source

model_LuminescenceSignals()

References

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

Examples

```
data(ExampleData.ModelOutput,envir = environment())
plot_RLum.Analysis(model.output)
```

---

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

`model`	`character` (**required**): set model to be used
`sequence`	`list` (**required**): set sequence to model as list or as *.seq file from the Riso sequence editor. To simulate SAR measurements there is an extra option to set the sequence list (cf. example 3): (**required**): RegDose: `numeric`, TestDose: `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
`plot`	`logical` (with default): Enables or disables plot output
`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

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, RLum.Analysis, RLum.Data.Curve

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(
  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 Gy) and simulate_sample_history = FALSE (default),
# because the sample history is not part of the sequence

model.output <- model_LuminescenceSignals(
   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(
 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 Gy) and simulate_sample_history = FALSE (default),
# because the sample history is not part of the sequence
```

```
 model.output <- model_LuminescenceSignals(

 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" (palaeodose = 10 Gy)
# and simulate_sample_history = FALSE (default),
# because the sample history is not part of the sequence

model.output <- model_LuminescenceSignals(
  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){

sequence <- 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)

##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)
```

`plot_concentrations` *Plot concentrations of electrones respectively holes of all levels from a energy-band-model against time.*

Description

The functions provides a plot of all changes in time of the electron respectively hole concentration in electron traps, hole centres, in the conduction and valence band.

Usage

```
plot_concentrations(object, record.step, ...)
```

Arguments

`object`	`RLum.Analysis` (**required**): S4 object of class `RLum.Analysis`, e.g. the values of `model_LuminescenceSignals`.
`record.step`	`numeric` (**required**): step of the simulated record which is to plot.
`...`	further arguments and graphical parameters passed to `plot.default`. See details for further information

Details

The function produces a multiple plot output and uses in main parts the Luminescence function "Luminescence::plot_RLum". A file output is recommended (e.g., `pdf`).

Value

Returns multiple plots for the concentrations of electrones respectively holes.

Function version

0.1.0

Author(s)

Johannes Friedrich, University of Bayreuth (Germany),

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`, `plot_RLum.Analysis`

Examples

```
##load data
data(ExampleData.ModelOutput, envir = environment())

##plot all concentrations
plot_concentrations(object = model.output, record.step = 1)

##plot only specific energy-band-level (e.g. 110 degree celsius trap, "concentration level 1")#'
plot_concentrations(object = model.output,
                    record.step = 1,
                    subset = list(recordType = "concentration level 1"))

##plot every level on a single plot
plot_concentrations(object = model.output, record.step = 1, plot.single = TRUE)
```

read_SEQ2R *Parse a Risoe SEQ-file to a sequence neccessary for simulating quartz luminescence*

Description

A SEQ-file created by the Risoe Sequence Editor can be imported to simulate the sequence written in the sequence editor.

Usage

```
read_SEQ2R(file, lab.DoseRate = 1, txtProgressBar = TRUE)
```

Arguments

`file`	`character` (**required**): a *.seq file created by the Risoe Sequene Editor
`lab.DoseRate`	`character` (with default): set the doserate of the radiation source in the laboratory [Gy/s]. Default: 1 Gy/s
`txtProgressBar`	`logical`: enables or disables the txtProgressBar
`...`	further arguments and graphical parameters passed to `plot.default`. See details for further information

Details

Supported versions

Suppored and tested: version 4.36.

Value

This function returns a list with the parsed *.seq file and the required steps for `model_LuminescenceSignals`

Function version

0.1.0

Author(s)

Johannes Friedrich, University of Bayreuth (Germany),

See Also

`plot`, `model_LuminescenceSignals`, `readLines`

Examples

```
#so far no example available
```

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