

Package ‘RLumModel’

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Type Package

Title Solving Ordinary Differential Equations to Understand
Luminescence

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Author Johannes Friedrich [aut, trl, cre],
Sebastian Kreutzer [aut, ths],
Christoph Schmidt [aut, ths]

Maintainer Johannes Friedrich <johannes.friedrich@uni-bayreuth.de>

Description A collection of functions to simulate luminescence sig-
nals in quartz and Al₂O₃ based on published models.

Contact Package Developer Team <developer@model.r-luminescence.de>

License GPL-3

Depends R (>= 3.3.0), utils, Luminescence (>= 0.7.0)

Imports deSolve (>= 1.12), methods, Rcpp

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RoxygenNote 6.0.1

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VignetteBuilder knitr

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RLumModel-package	<i>Solving Ordinary Differential Equations to Understand Luminescence</i>
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Description

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

Details

Package: RLumModel
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Author(s)

Authors

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

Supervisor

Christoph Schmidt, University of Bayreuth, Germany
 Sebastian Kreutzer, IRAMAT-CRP2A, Universite Bordeaux Montaigne, France

Support contact

<developers@model.r-luminescence.de>

Project source code repository

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

Related package projects

<http://www.r-luminescence.de>
<https://cran.r-project.org/package=Luminescence>
<http://shiny.r-luminescence.de>
<https://cran.r-project.org/package=RLumShiny>

Package maintainer

Johannes Friedrich, University of Bayreuth, Germany
<johannes.friedrich@uni-bayreuth.de>

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ExampleData.ModelOutput

Example data (TL curve) simulated with parameter set from Pagonis 2007

Description

Example data (TL curve) simulated with parameter set from Pagonis 2007

Format

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

Function version

0.1.1

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))`

Author(s)

Johannes Friedrich, University of Bayreuth (Germany)

Source

`model_LuminescenceSignals()`

References

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.

Examples

```
data("ExampleData.ModelOutput", envir = environment())

TL_curve <- get_RLum(model.output, recordType = "TL$", drop = FALSE)

##plot TL curve
plot_RLum(TL_curve)

TL_concentrations <- get_RLum(model.output, recordType = "(TL)", drop = FALSE)
plot_RLum(TL_concentrations)
```

```
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 defined 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.dose_rate = 1,
  simulate_sample_history = FALSE, plot = TRUE, verbose = TRUE,
  show_structure = FALSE, own_parameters = NULL,
  own_state_parameters = NULL, own_start_temperature = NULL, ...)
```

Arguments

model	character (required): set model to be used. Available models are: "Bailey2001", "Bailey2002", "Bailey2004", "Pagonis2007", "Pagonis2008", "Friedrich2017", "Friedrich2018" and for own models "customized" (or "customised"). Note: When model = "customized" is set, the argument 'own_parameters' has to be set.
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. details).
lab.dose_rate	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 laboratory 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
show_structure	logical (with default): Shows the structure of the result. Recommended to show record.id to analyse concentrations.
own_parameters	<p>list (with default): This argument allows the user to submit own parameter sets. The list has to contain the following items:</p> <ul style="list-style-type: none"> • N: Concentration of electron- and hole traps [cm^{-3}] • E: Electron/Hole trap depth [eV] • s: Frequency factor [s^{-1}] • A: Conduction band to electron trap and valence band to hole trap transition probability [$\text{s}^{-1} * \text{cm}^3$]. CAUTION: Not every publication uses the same definition of parameter A and B! See vignette "RLumModel - Usage with own parameter sets" for further details • B: Conduction band to hole centre transition probability [$\text{s}^{-1} * \text{cm}^3$]. • Th: Photo-eviction constant or photoionisation cross section, respectively • E_th: Thermal assistance energy [eV] • k_B: Boltzman constant $8.617\text{e-}05$ [eV/K] • W: activation energy 0.64 [eV] (for UV) • K: $2.8\text{e}7$ (dimensionless constant) • model: "customized" • R (optional): Ionisation rate (pair production rate) equivalent to 1 Gy/s [$\text{s}^{-1} * \text{cm}^{-3}$] <p>For further details see Bailey 2001, Wintle 1975, vignette "RLumModel - Using own parameter sets" and example 3.</p>
own_state_parameters	numeric (with default): Some publications (e.g. Pagonis 2009) offer state parameters. With this argument the user can submit this state parameters. For further details see vignette "RLumModel - Using own parameter sets" and example 3.
own_start_temperature	numeric (with default): Parameter to control the start temperature (in deg. C) of a simulation. This parameter takes effect only when 'model = "customized"' is choosen.
...	further arguments and graphical parameters passed to <code>plot.default</code> . See details for further information.

Details

Defining a **sequence**

Arguments	Description	Sub-arguments
-----------	-------------	---------------

TL	thermally stimulated luminescence	'temp begin' [°C], 'temp end' [°C], 'heating rate' [°C/s]
OSL	optically stimulated luminescence	'temp' [°C], 'duration' [s], 'optical_power' [%]
ILL	illumination	'temp' [°C], 'duration' [s], 'optical_power' [%]
LM_OSL	linear modulated OSL	'temp' [°C], 'duration' [s], optional: 'start_power' [%], 'end_power' [%]
RL/RF	radioluminescence	'temp' [°C], 'dose' [Gy], 'dose_rate' [Gy/s]
RF_heating	RF during heating/cooling	'temp begin' [°C], 'temp end' [°C], 'heating rate' [°C/s], 'dose_rate' [Gy/s]
IRR	irradiation	'temp' [°C], 'dose' [Gy], 'dose_rate' [Gy/s]
CH	cutheat	'temp' [°C], optional: 'duration' [s], 'heating_rate' [°C/s]
PH	preheat	'temp' [°C], 'duration' [s], optional: 'heating_rate' [°C/s]
PAUSE	pause	'temp' [°C], 'duration' [s]

Note: 100 % illumination power equates to 20 mW/cm²

Defining a **SAR-sequence**

Abrivation	Description	examples
RegDose	Dose points of the regenerative cycles [Gy]	c(0, 80, 140, 260, 320, 0, 80)
TestDose	Test dose for the SAR cycles [Gy]	50
PH	Temperature of the preheat [°C]	240
CH	Temperature of the cutheat [°C]	200
OSL_temp	Temperature of OSL read out [°C]	125
OSL_duration	Duration of OSL read out [s]	default: 40
Irr_temp	Temperature of irradiation [°C]	default: 20
PH_duration	Duration of the preheat [s]	default: 10
dose_rate	Dose rate of the laboratory irradiation source [Gy/s]	default: 1
optical_power	Percentage of the full illumination power [%]	default: 90
Irr_2recover	Dose to be recovered in a dose-recovery-test [Gy]	20

Value

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

Function version

0.1.5 (2017-11-20 14:14:40)

Author(s)

Johannes Friedrich, University of Bayreuth (Germany), Sebastian Kreutzer, IRAMAT-CRP2A, Université 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 its implications for the precision and accuracy of optical dating. *Radiation Measurements* 38, 299-310.
- Friedrich, J., Kreutzer, S., Schmidt, C., 2016. Solving ordinary differential equations to understand luminescence: 'RLumModel', an advanced research tool for simulating luminescence in quartz using R. *Quaternary Geochronology* 35, 88-100.
- Friedrich, J., Pagonis, V., Chen, R., Kreutzer, S., Schmidt, C., 2017: Quartz radiofluorescence: a modelling approach. *Journal of Luminescence* 186, 318-325.
- 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.
- Pagonis, V., Lawless, J., Chen, R., Anderson, C., 2009. Radioluminescence in Al₂O₃:C - analytical and numerical simulation results. *Journal of Physics D: Applied Physics* 42, 175107 (9pp).
- Soetaert, K., Cash, J., Mazzia, F., 2012. Solving differential equations in R. Springer Science & Business Media.
- Wintle, A., 1975. Thermal Quenching of Thermoluminescence in Quartz. *Geophysical Journal International* 41, 107-113.

See Also

[plot](#), [RLum](#), [read_SEQ2R](#)

Examples

```
##=====##
## Example 1: Simulate 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"
  )

  ##get all TL concentrations

  TL_conc <- get_RLum(model.output, recordType = "(TL)", drop = FALSE)

  plot_RLum(TL_conc)

  ##plot 110 deg. C trap concentration

  TL_110 <- get_RLum(TL_conc, recordType = "conc. level 1")
  plot_RLum(TL_110)

  ##=====##
  ## Example 2: 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(optical_power, function(x){

    sequence <- list(IRR = c(20, 50, 1),
                      PH = c(220, 10, 5),
                      OSL = c(125, 50, x)
                    )

    data <- model_LuminescenceSignals(
      sequence = sequence,
      model = "Bailey2004",
      plot = FALSE,
      verbose = FALSE
    )

    return(get_RLum(data, recordType = "OSL$", drop = 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)

```



```

##=====##
## Example 3: Usage of own parameter sets (Pagonis 2009)
##=====##

own_parameters <- list(
  N = c(2e15, 2e15, 1e17, 2.4e16),
  E = c(0, 0, 0, 0),
  s = c(0, 0, 0, 0),
  A = c(2e-8, 2e-9, 4e-9, 1e-8),
  B = c(0, 0, 5e-11, 4e-8),
  Th = c(0, 0),
  E_th = c(0, 0),
  k_B = 8.617e-5,
  W = 0.64,
  K = 2.8e7,
  model = "customized",
  R = 1.7e15
)
## Note: In Pagonis 2009 is B the valence band to hole centre probability,
## but in Bailey 2001 this is A_j. So the values of B (in Pagonis 2009)
## are A in the notation above. Also notice that the first two entries in N, A and
## B belong to the electron traps and the last two entries to the hole centres.

own_state_parameters <- c(0, 0, 0, 9.4e15)

## calculate Fig. 3 in Pagonis 2009. Note: The labels for the dose rate in the original
## publication are not correct.
## For a dose rate of 0.1 Gy/s belongs a RF signal to ~ 1.5e14 (see Fig. 6).

sequence <- list(RF = c(20, 0.1, 0.1))

model_LuminescenceSignals(
  model = "customized",
  sequence = sequence,
  own_parameters = own_parameters,
  own_state_parameters = own_state_parameters)

## Not run:
##=====##
## Example 4: Simulate Thermal-Activation-Characteristics (TAC)
##=====##

##set temperature
act.temp <- seq(from = 80, to = 600, by = 20)

##loop over temperature
model.output <- vapply(X = act.temp, FUN = function(x) {

##set sequence, note: sequence includes sample history

```

```

sequence <- list(
  IRR = c(20, 1, 1e-11),
  IRR = c(20, 10, 1),
  PH = c(x, 1),
  IRR = c(20, 0.1, 1),
  TL = c(20, 150, 5)
)
##run simulation
temp <- model_LuminescenceSignals(
  sequence = sequence,
  model = "Pagonis2007",
  simulate_sample_history = TRUE,
  plot = FALSE,
  verbose = FALSE
)
## "TL$" for exact matching TL and not (TL)
TL_curve <- get_RLum(temp, recordType = "TL$")
##return max value in TL curve
return(max(get_RLum(TL_curve)[,2]))
}, FUN.VALUE = 1)

##plot results
plot(
  act.temp[-(1:3)],
  model.output[-(1:3)],
  type = "b",
  xlab = "Temperature [\u00B0C]",
  ylab = "TL [a.u.]"
)

#####
## Example 5: 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 6: generate sequence from *.seq file and run SAR simulation
#####

# load example *.SEQ file and construct a sequence.
# call function "model_LuminescenceSignals", load created sequence for sequence,
# set model = "Bailey2002" (palaeodose = 10 Gy)
# and simulate_sample_history = FALSE (default),
# because the sample history is not part of the sequence

path <- system.file("extdata", "example_SAR_cycle.SEQ", package="RLumModel")

sequence <- read_SEQ2R(file = path)

model.output <- model_LuminescenceSignals(
  sequence = sequence,
  model = "Bailey2001",
  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 = 301,
  background.integral.max = 401,
  dose.points = c(0,8,14,26,32,0,8),
  fit.method = "EXP")

print(get_RLum(results))

```

```

#####
## Example 7: Simulate sequence at laboratory without sample history
#####

##set sequence with the following steps
## (1) Irraditation at 20 deg. C with a dose of 100 Gy and a dose rate of 1 Gy/s
## (2) Preheat to 200 deg. C and hold for 10 s
## (3) LM-OSL at 125 deg. C. for 100 s
## (4) Cutheat at 200 dec. C.
## (5) Irraditation at 20 deg. C with a dose of 10 Gy and a dose rate of 1 Gy/s
## (6) Pause at 200 de. C. for 100 s
## (7) OSL at 125 deg. C for 100 s with 90 % optical power
## (8) Pause at 200 deg. C for 100 s
## (9) TL from 20-400 deg. C with a heat rate of 5 K/s
## (10) Radiofluorescence at 20 deg. C with a dose of 200 Gy and a dose rate of 0.01 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"
)

## End(Not run)

```

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.dose_rate = 1, txtProgressBar = TRUE)
```

Arguments

`file` **character (required)**: a *.seq file created by the Risoe Sequence Editor

`lab.dose_rate` **character** (with default): set the dose rate of the radiation source in the laboratory Gy/s. Default: 1 Gy/s

`txtProgressBar` **logical** (with default): enables or disables the txtProgressBar for a visuall control of the progress. Default: txtProgressBar = TRUE

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 (2017-10-13 13:46:59)

Author(s)

Johannes Friedrich, University of Bayreuth (Germany),

References

Riso: Sequence Editor User Manual. Available at: http://www.nutech.dtu.dk/english/-/media/Andre_Universitetsenheder/Nutech/SequenceEditor.ashx?la=da

See Also

`model_LuminescenceSignals`, `readLines`

Examples

```
##search "example_SAR_cycle.SEQ" in "extdata" in package "RLumModel"
path <- system.file("extdata", "example_SAR_cycle.SEQ", package="RLumModel")

sequence <- read_SEQ2R(file = path, txtProgressBar = FALSE)
```

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