Package 'RLumModel'

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Type Package

Title Solving Ordinary Differential Equations to Understand Luminescence

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

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License GPL-3

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Luminescence (>= 0.7.0)

Imports deSolve (>= 1.12),
methods,
Rcpp

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`RLumModel-package` *Solving Ordinary Differential Equations to Unterstand Luminescence*

Description

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

Details

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Author(s)

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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

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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 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.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` `list` (with default): This argument allows the user to submit own parameter sets. The `list` has to contain the following items:

- 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 [s^(-1) * 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 [s^(-1) * cm^(3)].
- Th: Photo-eviction constant or photoionisation cross section, respectively
- E_th: Thermal assistence energy [eV]
- k_B: Boltzman constant 8.617e-05 [eV/K]
- W: activation energy 0.64 [eV] (for UV)
- K: 2.8e7 (dimensionless constant)
- model: "customized"
- R (optional): Ionisation rate (pair production rate) equivalent to 1 Gy/s [s^(-1) * cm^(-3)]

For further details see Bailey 2001, Wintle 1975, vignette "RLumModel - Using own parameter sets" and example 3.

`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 `plot.default`. 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'
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/cm^2

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

How to cite

Friedrich, J., Kreutzer, S. (2019). model_LuminescenceSignals(): Model Luminescence Signals. Function version 0.1.5. In: Friedrich, J., Kreutzer, S., Schmidt, C. (2019). RLumModel: Solving Ordinary Differential Equations to Understand LuminescenceR package version 0.2.4.9000-16. https://CRAN.R-project.org/package=RLumModel

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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.

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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 resutls
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 visuell control of the progress. Default: txtProgressBar = TRUE

Details

Supported versions: Supppored 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

How to cite

Friedrich, J. (2019). read_SEQ2R(): Parse a Risoe SEQ-file to a sequence neccessary for simulating quartz luminescence. Function version 0.1.0. In: Friedrich, J., Kreutzer, S., Schmidt, C. (2019). RLumModel: Solving Ordinary Differential Equations to Understand LuminescenceR package version 0.2.4.9000-16. https://CRAN.R-project.org/package=RLumModel

Author(s)

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References

Riso: Sequence Editor User Manual. Available at: http://www.nutech.dtu.dk/english/-/media/Andre_Universitetsenheder
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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